

Diisopropyl glutarate

Other names:	bis(1-methylethyl) pentanedioate glutaric acid, diisopropyl ester pentanedioic acid, bis(1-methylethyl) ester
Inchi:	InChI=1S/C11H20O4/c1-8(2)14-10(12)6-5-7-11(13)15-9(3)4/h8-9H,5-7H2,1-4H3
InchiKey:	MSQKMFJFBXZNQ-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CC(C)OC(=O)CCCC(=O)OC(C)C
Mol. weight [g/mol]:	216.27
CAS:	71340-46-0

Physical Properties

Property code	Value	Unit	Source
gf	-430.98	kJ/mol	Joback Method
hf	-770.53	kJ/mol	Joback Method
hfus	72.63	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	69.50	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	69.70	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	70.17	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	70.53	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	70.88	kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids

hfus	71.23		kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	71.59		kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	69.15		kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	72.28		kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	72.98		kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hfus	71.94		kJ/mol	Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids
hvap	57.62		kJ/mol	Joback Method
log10ws	-2.38			Crippen Method
logp	2.060			Crippen Method
mcvol	180.730		ml/mol	McGowan Method
pc	2131.49		kPa	Joback Method
rinpol	1322.00			NIST Webbook
rinpol	1322.00			NIST Webbook
rinpol	1317.00			NIST Webbook
rinpol	1321.00			NIST Webbook
rinpol	1323.00			NIST Webbook
rinpol	1323.00			NIST Webbook
rinpol	1319.00			NIST Webbook
tb	602.78		K	Joback Method
tc	787.66		K	Joback Method
tf	328.05		K	Joback Method
vc	0.688		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	465.83	J/molxK	602.78	Joback Method
cpg	531.86	J/molxK	756.85	Joback Method
cpg	519.94	J/molxK	726.03	Joback Method
cpg	507.38	J/molxK	695.22	Joback Method
cpg	494.18	J/molxK	664.41	Joback Method
cpg	480.33	J/molxK	633.59	Joback Method
cpg	543.12	J/molxK	787.66	Joback Method
dvisc	0.0001484	Paxs	602.78	Joback Method
dvisc	0.0001992	Paxs	556.99	Joback Method
dvisc	0.0002818	Paxs	511.20	Joback Method
dvisc	0.0004269	Paxs	465.41	Joback Method
dvisc	0.0007082	Paxs	419.63	Joback Method
dvisc	0.0013297	Paxs	373.84	Joback Method
dvisc	0.0029767	Paxs	328.05	Joback Method

Sources

Vapour pressure and enthalpy of vaporization of di-iso-propyl and di-tert-butyl esters of dicarboxylic acids:

McGowan Method:

NIST Webbook:

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1016/j.fluid.2011.07.007>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C71340460&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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