

Diethylmalonic acid, diisopropyl ester

Inchi:	InChI=1S/C13H24O4/c1-7-13(8-2,11(14)16-9(3)4)12(15)17-10(5)6/h9-10H,7-8H2,1-6H3
InchiKey:	SRBHXXKTKUSCB-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CCC(CC)(C(=O)OC(C)C)C(=O)OC(C)C
Mol. weight [g/mol]:	244.33

Physical Properties

Property code	Value	Unit	Source
gf	-411.30	kJ/mol	Joback Method
hf	-820.56	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.696		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	1287.00		NIST Webbook
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tb	645.31	K	Joback Method
tc	835.59	K	Joback Method
tf	353.01	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.06	J/molxK	645.31	Joback Method
cpg	644.77	J/molxK	803.87	Joback Method
cpg	631.88	J/molxK	772.16	Joback Method
cpg	618.18	J/molxK	740.45	Joback Method
cpg	603.65	J/molxK	708.74	Joback Method
cpg	588.28	J/molxK	677.02	Joback Method
cpg	656.88	J/molxK	835.59	Joback Method
dvisc	0.0001013	Paxs	645.31	Joback Method

dvisc	0.0001406	Paxs	596.59	Joback Method
dvisc	0.0002067	Paxs	547.88	Joback Method
dvisc	0.0003278	Paxs	499.16	Joback Method
dvisc	0.0005741	Paxs	450.44	Joback Method
dvisc	0.0011521	Paxs	401.73	Joback Method
dvisc	0.0028022	Paxs	353.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370280&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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