

Glutaric acid, ethyl neopentyl ester

Inchi:	InChI=1S/C12H22O4/c1-5-15-10(13)7-6-8-11(14)16-9-12(2,3)4/h5-9H2,1-4H3
InchiKey:	BIBNLWLYFRCTPS-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCOC(=O)CCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	230.30

Physical Properties

Property code	Value	Unit	Source
gf	-414.84	kJ/mol	Joback Method
hf	-789.36	kJ/mol	Joback Method
hfus	25.00	kJ/mol	Joback Method
hvap	59.32	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.309		Crippen Method
mvol	194.820	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1490.00		NIST Webbook
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tb	623.31	K	Joback Method
tc	809.02	K	Joback Method
tf	371.74	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.96	J/molxK	623.31	Joback Method
cpg	534.07	J/molxK	654.26	Joback Method
cpg	548.44	J/molxK	685.21	Joback Method
cpg	562.07	J/molxK	716.16	Joback Method
cpg	574.97	J/molxK	747.12	Joback Method
cpg	587.16	J/molxK	778.07	Joback Method
cpg	598.65	J/molxK	809.02	Joback Method
dvisc	0.0018446	Paxs	371.74	Joback Method

dvisc	0.0009542	Paxs	413.67	Joback Method
dvisc	0.0005573	Paxs	455.60	Joback Method
dvisc	0.0003563	Paxs	497.52	Joback Method
dvisc	0.0002443	Paxs	539.45	Joback Method
dvisc	0.0001768	Paxs	581.38	Joback Method
dvisc	0.0001337	Paxs	623.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358339&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
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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