

Glutaric acid, neopentyl octyl ester

Inchi:	InChI=1S/C18H34O4/c1-5-6-7-8-9-10-14-21-16(19)12-11-13-17(20)22-15-18(2,3)4/h5-15
InchiKey:	DJRGJEGONYGDMC-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCCCCCCOC(=O)CCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	314.46

Physical Properties

Property code	Value	Unit	Source
gf	-364.32	kJ/mol	Joback Method
hf	-913.20	kJ/mol	Joback Method
hfus	40.54	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.650		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinqol	2081.00		NIST Webbook
tb	760.59	K	Joback Method
tc	943.17	K	Joback Method
tf	439.36	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.04	J/molxK	760.59	Joback Method
cpg	929.42	J/molxK	912.74	Joback Method
cpg	915.57	J/molxK	882.31	Joback Method
cpg	900.82	J/molxK	851.88	Joback Method
cpg	885.17	J/molxK	821.45	Joback Method
cpg	868.59	J/molxK	791.02	Joback Method
cpg	942.42	J/molxK	943.17	Joback Method
dvisc	0.0000577	Paxs	760.59	Joback Method
dvisc	0.0000777	Paxs	707.05	Joback Method

dvisc	0.0001097	Paxs	653.51	Joback Method
dvisc	0.0001649	Paxs	599.97	Joback Method
dvisc	0.0002684	Paxs	546.44	Joback Method
dvisc	0.0004855	Paxs	492.90	Joback Method
dvisc	0.0010148	Paxs	439.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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