

Glutaric acid, neopentyl nonyl ester

Inchi:	InChI=1S/C19H36O4/c1-5-6-7-8-9-10-11-15-22-17(20)13-12-14-18(21)23-16-19(2,3)4/h5
InchiKey:	ZEFJBWFSTDJCRQ-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	328.49

Physical Properties

Property code	Value	Unit	Source
gf	-355.90	kJ/mol	Joback Method
hf	-933.84	kJ/mol	Joback Method
hfus	43.13	kJ/mol	Joback Method
hvap	74.90	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.040		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2176.00		NIST Webbook
tb	783.47	K	Joback Method
tc	967.35	K	Joback Method
tf	450.63	K	Joback Method
vc	1.137	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.17	J/mol×K	783.47	Joback Method
cpg	928.06	J/mol×K	814.12	Joback Method
cpg	944.94	J/mol×K	844.76	Joback Method
cpg	960.85	J/mol×K	875.41	Joback Method
cpg	975.81	J/mol×K	906.05	Joback Method
cpg	989.85	J/mol×K	936.70	Joback Method
cpg	1003.00	J/mol×K	967.35	Joback Method
dvisc	0.0009035	Paxs	450.63	Joback Method
dvisc	0.0004275	Paxs	506.10	Joback Method

dvisc	0.0002345	Paxs	561.58	Joback Method
dvisc	0.0001433	Paxs	617.05	Joback Method
dvisc	0.0000950	Paxs	672.52	Joback Method
dvisc	0.0000670	Paxs	728.00	Joback Method
dvisc	0.0000497	Paxs	783.47	Joback Method

Sources

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=U358347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	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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