

Glutaric acid, cyclohexylmethyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C18H32O4/c1-4-16(14(2)3)22-18(20)12-8-11-17(19)21-13-15-9-6-5-7-10-15/h1
InchiKey:	CIOMHFQCOAULQB-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	CCC(OC(=O)CCCC(=O)OCC1CCCCC1)C(C)C
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-347.59	kJ/mol	Joback Method
hf	-860.69	kJ/mol	Joback Method
hfus	32.74	kJ/mol	Joback Method
hvap	73.63	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.258		Crippen Method
mvol	268.500	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2121.00		NIST Webbook
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tb	782.49	K	Joback Method
tc	981.92	K	Joback Method
tf	414.32	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.94	J/molxK	782.49	Joback Method
cpg	866.02	J/molxK	815.73	Joback Method
cpg	883.83	J/molxK	848.97	Joback Method
cpg	900.38	J/molxK	882.21	Joback Method
cpg	915.68	J/molxK	915.44	Joback Method
cpg	929.77	J/molxK	948.68	Joback Method
cpg	942.65	J/molxK	981.92	Joback Method
dvisc	0.0017533	Paxs	414.32	Joback Method

dvisc	0.0007016	Paxs	475.68	Joback Method
dvisc	0.0003461	Paxs	537.04	Joback Method
dvisc	0.0001974	Paxs	598.40	Joback Method
dvisc	0.0001249	Paxs	659.77	Joback Method
dvisc	0.0000855	Paxs	721.13	Joback Method
dvisc	0.0000621	Paxs	782.49	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=U393498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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