

Glutaric acid, (cyclohex-3-enyl)methyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C18H30O4/c1-4-16(14(2)3)22-18(20)12-8-11-17(19)21-13-15-9-6-5-7-10-15/h5
InchiKey:	VSPOLMTUPQAHHX-UHFFFAOYSA-N
Formula:	C18H30O4
SMILES:	CCC(OC(=O)CCCC(=O)OCC1CC=CCC1)C(C)C
Mol. weight [g/mol]:	310.43

Physical Properties

Property code	Value	Unit	Source
gf	-317.63	kJ/mol	Joback Method
hf	-802.91	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	73.92	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.034		Crippen Method
mcvol	264.200	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2126.00		NIST Webbook
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tb	781.65	K	Joback Method
tc	982.14	K	Joback Method
tf	415.08	K	Joback Method
vc	0.999	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.23	J/molxK	781.65	Joback Method
cpg	838.52	J/molxK	815.06	Joback Method
cpg	855.56	J/molxK	848.48	Joback Method
cpg	871.39	J/molxK	881.89	Joback Method
cpg	886.02	J/molxK	915.31	Joback Method
cpg	899.47	J/molxK	948.72	Joback Method
cpg	911.76	J/molxK	982.14	Joback Method
dvisc	0.0016542	Paxs	415.08	Joback Method

dvisc	0.0006863	Paxs	476.18	Joback Method
dvisc	0.0003478	Paxs	537.27	Joback Method
dvisc	0.0002025	Paxs	598.37	Joback Method
dvisc	0.0001303	Paxs	659.46	Joback Method
dvisc	0.0000904	Paxs	720.56	Joback Method
dvisc	0.0000664	Paxs	781.65	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=U405525&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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