

Glutaric acid, cyclohexylmethyl cis-hex-3-enyl ester

Inchi:	InChI=1S/C18H30O4/c1-2-3-4-8-14-21-17(19)12-9-13-18(20)22-15-16-10-6-5-7-11-16/h3
InchiKey:	QTYYKNWRABMOKX-ARJAWSKDSA-N
Formula:	C18H30O4
SMILES:	CCC=CCCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	310.43

Physical Properties

Property code	Value	Unit	Source
gf	-262.49	kJ/mol	Joback Method
hf	-732.91	kJ/mol	Joback Method
hfus	39.99	kJ/mol	Joback Method
hvap	74.36	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.180		Crippen Method
mvol	264.200	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	787.53	K	Joback Method
tc	987.34	K	Joback Method
tf	439.24	K	Joback Method
vc	1.004	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.16	J/molxK	787.53	Joback Method
cpg	900.47	J/molxK	954.04	Joback Method
cpg	886.86	J/molxK	920.74	Joback Method
cpg	872.16	J/molxK	887.44	Joback Method
cpg	856.33	J/molxK	854.13	Joback Method
cpg	839.34	J/molxK	820.83	Joback Method
cpg	913.01	J/molxK	987.34	Joback Method
dvisc	0.0000637	Paxs	787.53	Joback Method

dvisc	0.0000849	Paxs	729.48	Joback Method
dvisc	0.0001188	Paxs	671.43	Joback Method
dvisc	0.0001774	Paxs	613.38	Joback Method
dvisc	0.0002880	Paxs	555.34	Joback Method
dvisc	0.0005234	Paxs	497.29	Joback Method
dvisc	0.0011139	Paxs	439.24	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=U394028&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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