

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

Inchi:	InChI=1S/C16H28O4/c1-3-5-7-9-14-20-16(18)12-10-11-15(17)19-13-8-6-4-2/h5,7H,3-4,6
InchiKey:	PEPWHWIXSXIUSX-ALCCZGGFSA-N
Formula:	C16H28O4
SMILES:	CCC=CCCOC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-303.78	kJ/mol	Joback Method
hf	-745.95	kJ/mol	Joback Method
hfus	42.97	kJ/mol	Joback Method
hvap	69.48	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.790		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinqol	2001.00		NIST Webbook
tb	722.22	K	Joback Method
tc	902.85	K	Joback Method
tf	409.32	K	Joback Method
vc	0.960	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.41	J/molxK	722.22	Joback Method
cpg	726.47	J/molxK	752.33	Joback Method
cpg	741.71	J/molxK	782.43	Joback Method
cpg	756.16	J/molxK	812.54	Joback Method
cpg	769.83	J/molxK	842.64	Joback Method
cpg	782.74	J/molxK	872.75	Joback Method
cpg	794.90	J/molxK	902.85	Joback Method
dvisc	0.0011649	Paxs	409.32	Joback Method
dvisc	0.0005794	Paxs	461.47	Joback Method

dvisc	0.0003321	Paxs	513.62	Joback Method
dvisc	0.0002109	Paxs	565.77	Joback Method
dvisc	0.0001446	Paxs	617.92	Joback Method
dvisc	0.0001051	Paxs	670.07	Joback Method
dvisc	0.0000801	Paxs	722.22	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=U359965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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