

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

Inchi:	InChI=1S/C13H22O4/c1-3-5-6-7-11-17-13(15)10-8-9-12(14)16-4-2/h5-6H,3-4,7-11H2,1-2
InchiKey:	SEEBGLPCIYCXHS-WAYWQWQ TSA-N
Formula:	C13H22O4
SMILES:	CCC=CCCOC(=O)CCCC(=O)OCC
Mol. weight [g/mol]:	242.31

Physical Properties

Property code	Value	Unit	Source
gf	-329.04	kJ/mol	Joback Method
hf	-684.03	kJ/mol	Joback Method
hfus	35.20	kJ/mol	Joback Method
hvap	62.80	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.619		Crippen Method
mvol	204.610	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
rinpol	1705.00		NIST Webbook
tb	653.58	K	Joback Method
tc	835.79	K	Joback Method
tf	375.51	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.88	J/molxK	653.58	Joback Method
cpg	561.52	J/molxK	683.95	Joback Method
cpg	575.46	J/molxK	714.32	Joback Method
cpg	588.72	J/molxK	744.69	Joback Method
cpg	601.30	J/molxK	775.06	Joback Method
cpg	613.22	J/molxK	805.43	Joback Method
cpg	624.48	J/molxK	835.79	Joback Method
dvisc	0.0014825	Paxs	375.51	Joback Method
dvisc	0.0007681	Paxs	421.85	Joback Method

dvisc	0.0004533	Paxs	468.20	Joback Method
dvisc	0.0002942	Paxs	514.54	Joback Method
dvisc	0.0002051	Paxs	560.89	Joback Method
dvisc	0.0001511	Paxs	607.23	Joback Method
dvisc	0.0001162	Paxs	653.58	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=U359961&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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