

Glutaric acid, cyclohexylmethyl tridecyl ester

Inchi:	InChI=1S/C25H46O4/c1-2-3-4-5-6-7-8-9-10-11-15-21-28-24(26)19-16-20-25(27)29-22-23
InchiKey:	FERWKTOQZWVDQO-UHFFFAOYSA-N
Formula:	C25H46O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	410.63

Physical Properties

Property code	Value	Unit	Source
gf	-283.77	kJ/mol	Joback Method
hf	-994.61	kJ/mol	Joback Method
hfus	57.91	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	7.134		Crippen Method
mcvol	367.130	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
rinpol	2994.00		NIST Webbook
rinpol	2994.00		NIST Webbook
tb	943.53	K	Joback Method
tc	1155.19	K	Joback Method
tf	523.21	K	Joback Method
vc	1.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1278.44	J/molxK	943.53	Joback Method
cpg	1360.98	J/molxK	1119.92	Joback Method
cpg	1347.60	J/molxK	1084.64	Joback Method
cpg	1332.70	J/molxK	1049.36	Joback Method
cpg	1316.24	J/molxK	1014.08	Joback Method
cpg	1298.16	J/molxK	978.81	Joback Method
cpg	1372.89	J/molxK	1155.19	Joback Method
dvisc	0.0000259	Paxs	943.53	Joback Method

dvisc	0.0000349	Paxs	873.48	Joback Method
dvisc	0.0000497	Paxs	803.42	Joback Method
dvisc	0.0000755	Paxs	733.37	Joback Method
dvisc	0.0001254	Paxs	663.32	Joback Method
dvisc	0.0002350	Paxs	593.26	Joback Method
dvisc	0.0005206	Paxs	523.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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