

Glutaric acid, cyclohexylmethyl dodecyl ester

Inchi: InChI=1S/C24H44O4/c1-2-3-4-5-6-7-8-9-10-14-20-27-23(25)18-15-19-24(26)28-21-22-16
InchiKey: AEHJAJFTCRORIH-UHFFFAOYSA-N
Formula: C24H44O4
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-292.19	kJ/mol	Joback Method
hf	-973.97	kJ/mol	Joback Method
hfus	55.32	kJ/mol	Joback Method
hvap	87.76	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.744		Crippen Method
mvol	353.040	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	2868.00		NIST Webbook
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tb	920.65	K	Joback Method
tc	1127.37	K	Joback Method
tf	511.94	K	Joback Method
vc	1.361	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.01	J/molxK	920.65	Joback Method
cpg	1297.40	J/molxK	1092.92	Joback Method
cpg	1283.88	J/molxK	1058.46	Joback Method
cpg	1268.92	J/molxK	1024.01	Joback Method
cpg	1252.48	J/molxK	989.56	Joback Method
cpg	1234.53	J/molxK	955.10	Joback Method
cpg	1309.52	J/molxK	1127.37	Joback Method
dvisc	0.0000302	Paxs	920.65	Joback Method

dvisc	0.0000407	Paxs	852.53	Joback Method
dvisc	0.0000577	Paxs	784.41	Joback Method
dvisc	0.0000875	Paxs	716.29	Joback Method
dvisc	0.0001447	Paxs	648.18	Joback Method
dvisc	0.0002695	Paxs	580.06	Joback Method
dvisc	0.0005921	Paxs	511.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391598&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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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