

Glutaric acid, cyclohexylmethyl nonyl ester

Inchi: InChI=1S/C21H38O4/c1-2-3-4-5-6-7-11-17-24-20(22)15-12-16-21(23)25-18-19-13-9-8-10
InchiKey: JKZKJTIPURQYHX-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: CCCCCCCCCOC(=O)CCCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-317.45	kJ/mol	Joback Method
hf	-912.05	kJ/mol	Joback Method
hfus	47.55	kJ/mol	Joback Method
hvap	81.08	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.574		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2576.00		NIST Webbook
rinpol	2576.00		NIST Webbook
tb	852.01	K	Joback Method
tc	1049.36	K	Joback Method
tf	478.13	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.64	J/molxK	852.01	Joback Method
cpg	1109.61	J/molxK	1016.47	Joback Method
cpg	1095.80	J/molxK	983.58	Joback Method
cpg	1080.72	J/molxK	950.68	Joback Method
cpg	1064.35	J/molxK	917.79	Joback Method
cpg	1046.67	J/molxK	884.90	Joback Method
cpg	1122.19	J/molxK	1049.36	Joback Method
dvisc	0.0000476	Paxs	852.01	Joback Method

dvisc	0.0000637	Paxs	789.70	Joback Method
dvisc	0.0000896	Paxs	727.38	Joback Method
dvisc	0.0001344	Paxs	665.07	Joback Method
dvisc	0.0002192	Paxs	602.76	Joback Method
dvisc	0.0004003	Paxs	540.44	Joback Method
dvisc	0.0008554	Paxs	478.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391518&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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