

Glutaric acid, 8-chlorooctyl trans-4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C23H41ClO4/c1-23(2,3)19-13-15-20(16-14-19)28-22(26)12-10-11-21(25)27-18
InchiKey:	NQYWJACVZRPXEI-UHFFFAOYSA-N
Formula:	C23H41ClO4
SMILES:	CC(C)(C)C1CCC(OC(=O)CCCC(=O)OCCCCCCCCCl)CC1
Mol. weight [g/mol]:	417.02

Physical Properties

Property code	Value	Unit	Source
gf	-317.41	kJ/mol	Joback Method
hf	-998.16	kJ/mol	Joback Method
hfus	50.59	kJ/mol	Joback Method
hvap	88.31	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.427		Crippen Method
mvol	351.190	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	3021.00		NIST Webbook
rinpol	3021.00		NIST Webbook
tb	927.30	K	Joback Method
tc	1137.63	K	Joback Method
tf	528.77	K	Joback Method
vc	1.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.18	J/molxK	927.30	Joback Method
cpg	1204.47	J/molxK	962.35	Joback Method
cpg	1221.25	J/molxK	997.41	Joback Method
cpg	1236.56	J/molxK	1032.46	Joback Method
cpg	1250.46	J/molxK	1067.52	Joback Method
cpg	1263.00	J/molxK	1102.57	Joback Method
cpg	1274.23	J/molxK	1137.63	Joback Method
dvisc	0.0005195	Paxs	528.77	Joback Method

dvisc	0.0002481	Paxs	595.19	Joback Method
dvisc	0.0001375	Paxs	661.61	Joback Method
dvisc	0.0000848	Paxs	728.03	Joback Method
dvisc	0.0000567	Paxs	794.46	Joback Method
dvisc	0.0000404	Paxs	860.88	Joback Method
dvisc	0.0000302	Paxs	927.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393408&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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