Glutaric acid, 3,4-dimethylcyclohexyl 8-chlorooctyl ester

Inchi: InChI=1S/C21H37ClO4/c1-17-12-13-19(16-18(17)2)26-21(24)11-9-10-20(23)25-15-8-6-4
InchiKey: BUZXPHIZMCGOLG-UHFFFAOYSA-N
Formula: C21H37ClO4
SMILES: CC1CCC(OC(=O)CCCC(=O)OCCCCCCCCCCl)CC1C
Mol. weight [g/mol]: 388.97

Physical Properties

Property code	Value	Unit	Source
gf	-344.80	kJ/mol	Joback Method
hf	-968.47	kJ/mol	Joback Method
hfus	53.89	kJ/mol	Joback Method
hvap	84.85	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.647		Crippen Method
mcvol	323.010	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook
tb	880.10	K	Joback Method
tc	1082.21	K	Joback Method
tf	499.57	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.81	J/mol×K	880.10	Joback Method
cpg	1084.16	J/mol×K	913.79	Joback Method
cpg	1101.03	J/mol×K	947.47	Joback Method
cpg	1116.45	J/mol×K	981.16	Joback Method
cpg	1130.42	J/mol×K	1014.84	Joback Method
cpg	1142.98	J/mol×K	1048.53	Joback Method
cpg	1154.13	J/mol×K	1082.21	Joback Method
dvisc	0.0007940	Pa×s	499.57	Joback Method

dvisc	0.0004199	Pa×s	562.99	Joback Method
dvisc	0.0002527	Pa×s	626.41	Joback Method
dvisc	0.0001669	Pa×s	689.84	Joback Method
dvisc	0.0001183	Pa×s	753.26	Joback Method
dvisc	0.0000884	Pa×s	816.68	Joback Method
dvisc	0.0000689	Pa×s	880.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U405433&Units=SI

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