Glutaric acid, 2,3-dichlorophenyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C21H30Cl2O4/c1-15(2)7-4-8-16(3)13-14-26-19(24)11-6-12-20(25)27-18-10-5-9

InchiKey: LUESKPZWMBPICL-UHFFFAOYSA-N

Formula: C21H30Cl2O4

SMILES: CC(C)CCCC(C)CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 417.37

Physical Properties

Property code	Value	Unit	Source
gf	-277.49	kJ/mol	Joback Method
hf	-794.82	kJ/mol	Joback Method
hfus	50.33	kJ/mol	Joback Method
hvap	92.25	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.465		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	2860.00		NIST Webbook
rinpol	2860.00		NIST Webbook
tb	943.08	K	Joback Method
tc	1159.39	K	Joback Method
tf	552.05	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.36	J/mol×K	943.08	Joback Method
cpg	1003.31	J/mol×K	979.13	Joback Method
cpg	1015.96	J/mol×K	1015.18	Joback Method
cpg	1027.34	J/mol×K	1051.23	Joback Method
cpg	1037.49	J/mol×K	1087.28	Joback Method
cpg	1046.42	J/mol×K	1123.33	Joback Method
cpg	1054.18	J/mol×K	1159.39	Joback Method
dvisc	0.0003700	Pa×s	552.05	Joback Method

dvisc	0.0001941	Pa×s	617.22	Joback Method
dvisc	0.0001151	Pa×s	682.39	Joback Method
dvisc	0.0000748	Pa×s	747.56	Joback Method
dvisc	0.0000521	Pa×s	812.74	Joback Method
dvisc	0.0000383	Pa×s	877.91	Joback Method
dvisc	0.0000294	Pa×s	943.08	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=U391490&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