Glutaric acid, 8-chlorooctyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C21H39ClO4/c1-18(16-21(2,3)4)17-26-20(24)13-11-12-19(23)25-15-10-8-6-5-7

InchiKey: GDJJJBABGNUWTQ-UHFFFAOYSA-N

Formula: C21H39ClO4

SMILES: CC(COC(=O)CCCC(=O)OCCCCCCCCCCl)CC(C)(C)C

Mol. weight [g/mol]: 390.99

Physical Properties

Property code	Value	Unit	Source
gf	-353.43	kJ/mol	Joback Method
hf	-996.14	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	83.35	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.895		Crippen Method
mcvol	333.870	ml/mol	McGowan Method
pc	1006.53	kPa	Joback Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
tb	866.22	K	Joback Method
tc	1062.30	K	Joback Method
tf	488.09	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.81	J/mol×K	866.22	Joback Method
cpg	1080.48	J/mol×K	898.90	Joback Method
cpg	1097.00	J/mol×K	931.58	Joback Method
cpg	1112.42	J/mol×K	964.26	Joback Method
cpg	1126.76	J/mol×K	996.94	Joback Method
cpg	1140.08	J/mol×K	1029.62	Joback Method
cpg	1152.40	J/mol×K	1062.30	Joback Method
dvisc	0.0006294	Pa×s	488.09	Joback Method

dvisc	0.0002789	Pa×s	551.11	Joback Method
dvisc	0.0001461	Pa×s	614.13	Joback Method
dvisc	0.0000863	Pa×s	677.15	Joback Method
dvisc	0.0000557	Pa×s	740.18	Joback Method
dvisc	0.0000386	Pa×s	803.20	Joback Method
dvisc	0.0000282	Pa×s	866.22	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=U391540&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