Glutaric acid, (2-methylcyclohex-1-enyl)methyl 8-chlorooctyl ester

Inchi: InChI=1S/C21H35ClO4/c1-18-11-6-7-12-19(18)17-26-21(24)14-10-13-20(23)25-16-9-5-3

InchiKey: QNCQLMUCTCGRIC-UHFFFAOYSA-N

Formula: C21H35ClO4

SMILES: CC1=C(COC(=O)CCCC(=O)OCCCCCCCCCCl)CCCC1

Mol. weight [g/mol]: 386.95

Physical Properties

Property code	Value	Unit	Source
gf	-310.97	kJ/mol	Joback Method
hf	-872.61	kJ/mol	Joback Method
hfus	51.12	kJ/mol	Joback Method
hvap	87.39	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.713		Crippen Method
mcvol	318.710	ml/mol	McGowan Method
pc	1160.87	kPa	Joback Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		NIST Webbook
tb	903.23	K	Joback Method
tc	1109.61	K	Joback Method
tf	538.09	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.76	J/mol×K	903.23	Joback Method
cpg	1040.34	J/mol×K	937.63	Joback Method
cpg	1055.61	J/mol×K	972.02	Joback Method
cpg	1069.60	J/mol×K	1006.42	Joback Method
cpg	1082.33	J/mol×K	1040.82	Joback Method
cpg	1093.83	J/mol×K	1075.21	Joback Method
cpg	1104.14	J/mol×K	1109.61	Joback Method
dvisc	0.0004338	Pa×s	538.09	Joback Method

dvisc	0.0002296	Pa×s	598.95	Joback Method
dvisc	0.0001367	Pa×s	659.80	Joback Method
dvisc	0.0000888	Pa×s	720.66	Joback Method
dvisc	0.0000617	Pa×s	781.52	Joback Method
dvisc	0.0000452	Pa×s	842.37	Joback Method
dvisc	0.0000345	Pa×s	903.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405509&Units=SI
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

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