Glutaric acid, 2-(cyclohexyl)ethyl 8-chlorooctyl ester

Inchi: InChI=1S/C21H37ClO4/c22-16-8-3-1-2-4-9-17-25-20(23)13-10-14-21(24)26-18-15-19-11

InchiKey: JSNLAVBCJUXCSZ-UHFFFAOYSA-N

Formula: C21H37ClO4

SMILES: O=C(CCCC(=O)OCCC1CCCCC1)OCCCCCCCCCl

Mol. weight [g/mol]: 388.97

Physical Properties

Property code	Value	Unit	Source
gf	-329.38	kJ/mol	Joback Method
hf	-927.79	kJ/mol	Joback Method
hfus	51.75	kJ/mol	Joback Method
hvap	85.47	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.793		Crippen Method
mcvol	323.010	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	2836.00		NIST Webbook
rinpol	2836.00		NIST Webbook
tb	889.44	K	Joback Method
tc	1092.90	K	Joback Method
tf	508.05	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.30	J/mol×K	889.44	Joback Method
cpg	1076.05	J/mol×K	923.35	Joback Method
cpg	1092.42	J/mol×K	957.26	Joback Method
cpg	1107.43	J/mol×K	991.17	Joback Method
cpg	1121.12	J/mol×K	1025.08	Joback Method
cpg	1133.52	J/mol×K	1058.99	Joback Method
cpg	1144.66	J/mol×K	1092.90	Joback Method
dvisc	0.0006650	Pa×s	508.05	Joback Method

dvisc	0.0003215	Pa×s	571.62	Joback Method
dvisc	0.0001798	Pa×s	635.18	Joback Method
dvisc	0.0001118	Pa×s	698.75	Joback Method
dvisc	0.0000752	Pa×s	762.31	Joback Method
dvisc	0.0000538	Pa×s	825.88	Joback Method
dvisc	0.0000404	Pa×s	889.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405422&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