Glutaric acid, cyclohexylmethyl 10-chlorodecyl ester

Inchi: InChI=1S/C22H39ClO4/c23-17-10-5-3-1-2-4-6-11-18-26-21(24)15-12-16-22(25)27-19-20

InchiKey: FLCMGNKTCRCPBB-UHFFFAOYSA-N

Formula: C22H39ClO4

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCCCCCCCCCCCCl

Mol. weight [g/mol]: 403.00

Physical Properties

Property code	Value	Unit	Source
gf	-320.96	kJ/mol	Joback Method
hf	-948.43	kJ/mol	Joback Method
hfus	54.34	kJ/mol	Joback Method
hvap	87.69	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.183		Crippen Method
mcvol	337.100	ml/mol	McGowan Method
pc	1061.02	kPa	Joback Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook
tb	912.32	K	Joback Method
tc	1118.67	K	Joback Method
tf	519.32	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.95	J/mol×K	912.32	Joback Method
cpg	1195.25	J/mol×K	1084.28	Joback Method
cpg	1182.96	J/mol×K	1049.89	Joback Method
cpg	1169.31	J/mol×K	1015.50	Joback Method
cpg	1154.29	J/mol×K	981.10	Joback Method
cpg	1137.84	J/mol×K	946.71	Joback Method
cpg	1206.24	J/mol×K	1118.67	Joback Method
dvisc	0.0000346	Pa×s	912.32	Joback Method

dvisc	0.0000462	Pa×s	846.82	Joback Method
dvisc	0.0000648	Pa×s	781.32	Joback Method
dvisc	0.0000966	Pa×s	715.82	Joback Method
dvisc	0.0001562	Pa×s	650.32	Joback Method
dvisc	0.0002813	Pa×s	584.82	Joback Method
dvisc	0.0005874	Pa×s	519.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392468&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

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