Glutaric acid, (2-chlorocyclohexyl)methyl dec-2-yl ester

Inchi: InChI=1S/C22H39ClO4/c1-3-4-5-6-7-8-12-18(2)27-22(25)16-11-15-21(24)26-17-19-13-9-

InchiKey: ZAXNSBLQUUUWPJ-UHFFFAOYSA-N

Formula: C22H39ClO4

SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)OCC1CCCCC1Cl

Mol. weight [g/mol]: 403.00

Physical Properties

Property code	Value	Unit	Source
gf	-331.11	kJ/mol	Joback Method
hf	-974.05	kJ/mol	Joback Method
hfus	51.89	kJ/mol	Joback Method
hvap	86.99	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.180		Crippen Method
mcvol	337.100	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
rinpol	2771.00		NIST Webbook
rinpol	2771.00		NIST Webbook
tb	907.21	K	Joback Method
tc	1113.50	K	Joback Method
tf	500.08	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.30	J/mol×K	907.21	Joback Method
cpg	1142.49	J/mol×K	941.59	Joback Method
cpg	1159.16	J/mol×K	975.97	Joback Method
cpg	1174.32	J/mol×K	1010.36	Joback Method
cpg	1188.03	J/mol×K	1044.74	Joback Method
cpg	1200.29	J/mol×K	1079.12	Joback Method
cpg	1211.13	J/mol×K	1113.50	Joback Method
dvisc	0.0007380	Pa×s	500.08	Joback Method

dvisc	0.0003432	Pa×s	567.94	Joback Method
dvisc	0.0001880	Pa×s	635.79	Joback Method
dvisc	0.0001156	Pa×s	703.64	Joback Method
dvisc	0.0000775	Pa×s	771.50	Joback Method
dvisc	0.0000554	Pa×s	839.35	Joback Method
dvisc	0.0000416	Pa×s	907.21	Joback Method

Sources

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=U405451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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