Glutaric acid, cyclohexylmethyl 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C19H25ClO4/c1-14-10-11-16(20)17(12-14)24-19(22)9-5-8-18(21)23-13-15-6-3

InchiKey: AXAUMGDYPICLTD-UHFFFAOYSA-N

Formula: C19H25ClO4

SMILES: Cc1ccc(Cl)c(OC(=O)CCCC(=O)OCC2CCCCC2)c1

Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-253.07	kJ/mol	Joback Method
hf	-672.92	kJ/mol	Joback Method
hfus	39.83	kJ/mol	Joback Method
hvap	84.61	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.848		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2659.00		NIST Webbook
rinpol	2659.00		NIST Webbook
tb	880.32	K	Joback Method
tc	1105.43	K	Joback Method
tf	536.97	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.57	J/mol×K	880.32	Joback Method
cpg	854.90	J/mol×K	917.84	Joback Method
cpg	868.74	J/mol×K	955.36	Joback Method
cpg	881.14	J/mol×K	992.88	Joback Method
cpg	892.11	J/mol×K	1030.40	Joback Method
cpg	901.69	J/mol×K	1067.91	Joback Method
cpg	909.89	J/mol×K	1105.43	Joback Method
dvisc	0.0005300	Pa×s	536.97	Joback Method

dvisc	0.0003060	Pa×s	594.20	Joback Method
dvisc	0.0001946	Pa×s	651.42	Joback Method
dvisc	0.0001331	Pa×s	708.64	Joback Method
dvisc	0.0000964	Pa×s	765.87	Joback Method
dvisc	0.0000730	Pa×s	823.10	Joback Method
dvisc	0.0000573	Pa×s	880.32	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=U393425&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