Glutaric acid, 2-(adamant-1-yl)ethyl 3-chlorophenyl ester

Inchi: InChI=1S/C23H29ClO4/c24-19-3-1-4-20(12-19)28-22(26)6-2-5-21(25)27-8-7-23-13-16-9-
InchiKey: MOATWNDIJLWAOI-UHFFFAOYSA-N
Formula: C23H29ClO4
SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 404.93

Physical Properties

Property code	Value	Unit	Source
gf	-77.26	kJ/mol	Joback Method
hf	-591.19	kJ/mol	Joback Method
hfus	45.83	kJ/mol	Joback Method
hvap	90.88	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.565		Crippen Method
mcvol	305.710	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	3196.00		NIST Webbook
rinpol	3196.00		NIST Webbook
tb	967.37	K	Joback Method
tc	1200.76	K	Joback Method
tf	632.11	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.94	J/mol×K	967.37	Joback Method
cpg	1066.04	J/mol×K	1006.27	Joback Method
cpg	1087.19	J/mol×K	1045.17	Joback Method
cpg	1108.64	J/mol×K	1084.06	Joback Method
cpg	1130.60	J/mol×K	1122.96	Joback Method
cpg	1153.34	J/mol×K	1161.86	Joback Method
cpg	1177.09	J/mol×K	1200.76	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=U405386&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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