Succinic acid, 4-chloro-3-methylphenyl adamant-2-yl ester

Inchi: InChI=1S/C21H25ClO4/c1-12-6-17(2-3-18(12)22)25-19(23)4-5-20(24)26-21-15-8-13-7-14

InchiKey: KGVNNGBANNXFLC-UHFFFAOYSA-N

Formula: C21H25ClO4

SMILES: Cc1cc(OC(=O)CCC(=O)OC2C3CC4CC(C3)CC2C4)ccc1Cl

Mol. weight [g/mol]: 376.87

Physical Properties

Property code	Value	Unit	Source
gf	-105.95	kJ/mol	Joback Method
hf	-596.96	kJ/mol	Joback Method
hfus	47.63	kJ/mol	Joback Method
hvap	87.93	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.702		Crippen Method
mcvol	277.530	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	3058.00		NIST Webbook
rinpol	3058.00		NIST Webbook
tb	921.68	K	Joback Method
tc	1152.99	K	Joback Method
tf	593.95	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.87	J/mol×K	921.68	Joback Method
cpg	994.68	J/mol×K	1114.44	Joback Method
cpg	982.44	J/mol×K	1075.89	Joback Method
cpg	969.35	J/mol×K	1037.34	Joback Method
cpg	955.29	J/mol×K	998.78	Joback Method
cpg	940.17	J/mol×K	960.23	Joback Method
cpg	1006.17	J/mol×K	1152.99	Joback Method
dvisc	0.0017108	Pa×s	921.68	Joback Method

dvisc	0.0018694	Pa×s	867.06	Joback Method
dvisc	0.0020672	Pa×s	812.44	Joback Method
dvisc	0.0023193	Pa×s	757.82	Joback Method
dvisc	0.0026490	Pa×s	703.19	Joback Method
dvisc	0.0030942	Pa×s	648.57	Joback Method
dvisc	0.0037190	Pa×s	593.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391349&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