Succinic acid, 3-chlorophenyl adamant-2-yl ester

Inchi: InChI=1S/C20H23ClO4/c21-16-2-1-3-17(11-16)24-18(22)4-5-19(23)25-20-14-7-12-6-13(9

InchiKey: MYTPUOPRBSBMIW-UHFFFAOYSA-N

Formula: C20H23ClO4

SMILES: O=C(CCC(=O)OC1C2CC3CC(C2)CC1C3)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 362.85

Physical Properties

Property code	Value	Unit	Source
gf	-104.74	kJ/mol	Joback Method
hf	-564.85	kJ/mol	Joback Method
hfus	45.43	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.393		Crippen Method
mcvol	263.440	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	2874.00		NIST Webbook
tb	893.82	K	Joback Method
tc	1126.23	K	Joback Method
tf	570.16	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.35	J/mol×K	893.82	Joback Method
cpg	881.63	J/mol×K	932.55	Joback Method
cpg	896.72	J/mol×K	971.29	Joback Method
cpg	910.73	J/mol×K	1010.02	Joback Method
cpg	923.78	J/mol×K	1048.76	Joback Method
cpg	935.97	J/mol×K	1087.49	Joback Method
cpg	947.41	J/mol×K	1126.23	Joback Method
dvisc	0.0040406	Pa×s	570.16	Joback Method
dvisc	0.0033410	Pa×s	624.10	Joback Method

dvisc	0.0028474	Pa×s	678.05	Joback Method
dvisc	0.0024846	Pa×s	731.99	Joback Method
dvisc	0.0022089	Pa×s	785.93	Joback Method
dvisc	0.0019937	Pa×s	839.88	Joback Method
dvisc	0.0018219	Pa×s	893.82	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=U391347&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