Succinic acid, 2-(adamant-1-yl)ethyl 8-chlorooctyl ester

Inchi: InChI=1S/C24H39ClO4/c25-10-5-3-1-2-4-6-11-28-22(26)7-8-23(27)29-12-9-24-16-19-13-
InchiKey: UBOOLNSNYCMHKP-UHFFFAOYSA-N
Formula: C24H39ClO4
SMILES: O=C(CCC(=O)OCCC12CC3CC(CC(C3)C1)C2)OCCCCCCCCCl
Mol. weight [g/mol]: 427.02

Physical Properties

Property code	Value	Unit	Source
gf	-171.62	kJ/mol	Joback Method
hf	-836.89	kJ/mol	Joback Method
hfus	54.76	kJ/mol	Joback Method
hvap	90.17	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	6.039		Crippen Method
mcvol	343.560	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
tb	958.59	K	Joback Method
tc	1175.33	K	Joback Method
tf	604.44	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1209.62	J/mol×K	958.59	Joback Method
cpg	1232.48	J/mol×K	994.71	Joback Method
cpg	1255.16	J/mol×K	1030.84	Joback Method
cpg	1277.88	J/mol×K	1066.96	Joback Method
cpg	1300.81	J/mol×K	1103.08	Joback Method
cpg	1324.17	J/mol×K	1139.20	Joback Method
cpg	1348.15	J/mol×K	1175.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391370&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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