Succinic acid, hexyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C15H26O4/c1-4-5-6-7-11-18-14(16)8-9-15(17)19-12-10-13(2)3/h2,4-12H2,1,3H
InchiKey: HWGFJLBAFBRGCO-UHFFFAOYSA-N
Formula: C15H26O4
SMILES: C=C(C)CCOC(=O)CCC(=O)OCCCCCC
Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-313.13	kJ/mol	Joback Method
hf	-726.89	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	66.71	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.399		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	1828.00		NIST Webbook
tb	691.74	K	Joback Method
tc	871.40	K	Joback Method
tf	387.41	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.06	J/mol×K	691.74	Joback Method
cpg	668.81	J/mol×K	721.68	Joback Method
cpg	683.78	J/mol×K	751.63	Joback Method
cpg	697.99	J/mol×K	781.57	Joback Method
cpg	711.44	J/mol×K	811.52	Joback Method
cpg	724.15	J/mol×K	841.46	Joback Method
cpg	736.13	J/mol×K	871.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353443&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
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