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

Inchi: InChI=1S/C17H30O4/c1-4-5-6-9-13-20-16(18)10-7-8-11-17(19)21-14-12-15(2)3/h2,4-14H
InchiKey: KBCFBEIHXYRCAZ-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-296.29	kJ/mol	Joback Method
hf	-768.17	kJ/mol	Joback Method
hfus	42.77	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.180		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2027.00		NIST Webbook
tb	737.50	K	Joback Method
tc	917.45	K	Joback Method
tf	409.95	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.49	J/mol×K	737.50	Joback Method
cpg	782.08	J/mol×K	767.49	Joback Method
cpg	797.81	J/mol×K	797.48	Joback Method
cpg	812.70	J/mol×K	827.48	Joback Method
cpg	826.76	J/mol×K	857.47	Joback Method
cpg	840.00	J/mol×K	887.46	Joback Method
cpg	852.44	J/mol×K	917.45	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=U354029&Units=SI

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