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

Inchi: InChI=1S/C17H30O4/c1-14(2)8-7-12-20-16(18)9-5-6-10-17(19)21-13-11-15(3)4/h14H,3,5
InchiKey: BRDXTCMREAPHGR-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-298.73	kJ/mol	Joback Method
hf	-773.45	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.036		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	1992.00		NIST Webbook
tb	737.06	K	Joback Method
tc	918.87	K	Joback Method
tf	394.95	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.98	J/mol×K	737.06	Joback Method
cpg	782.76	J/mol×K	767.36	Joback Method
cpg	798.65	J/mol×K	797.66	Joback Method
cpg	813.68	J/mol×K	827.96	Joback Method
cpg	827.85	J/mol×K	858.26	Joback Method
cpg	841.17	J/mol×K	888.56	Joback Method
cpg	853.67	J/mol×K	918.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354028&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