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

Inchi: InChI=1S/C14H24O4/c1-4-10-17-13(15)7-5-6-8-14(16)18-11-9-12(2)3/h2,4-11H2,1,3H3
InchiKey: IIAKZBOCMIGQCL-UHFFFAOYSA-N
Formula: C14H24O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCC
Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-321.55	kJ/mol	Joback Method
hf	-706.25	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	64.48	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.009		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
tb	668.86	K	Joback Method
tc	849.09	K	Joback Method
tf	376.14	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.65	J/mol×K	668.86	Joback Method
cpg	613.92	J/mol×K	698.90	Joback Method
cpg	628.46	J/mol×K	728.94	Joback Method
cpg	642.28	J/mol×K	758.98	Joback Method
cpg	655.38	J/mol×K	789.01	Joback Method
cpg	667.77	J/mol×K	819.05	Joback Method
cpg	679.46	J/mol×K	849.09	Joback Method

Sources

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=U354025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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