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

Inchi: InChI=1S/C16H28O4/c1-4-5-8-12-19-15(17)9-6-7-10-16(18)20-13-11-14(2)3/h2,4-13H2,1
InchiKey: UDDUVKRWIRAHCV-UHFFFAOYSA-N
Formula: C16H28O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCCCC
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-304.71	kJ/mol	Joback Method
hf	-747.53	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.790		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	1938.00		NIST Webbook
tb	714.62	K	Joback Method
tc	894.17	K	Joback Method
tf	398.68	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.70	J/mol×K	714.62	Joback Method
cpg	724.88	J/mol×K	744.55	Joback Method
cpg	740.25	J/mol×K	774.47	Joback Method
cpg	754.81	J/mol×K	804.40	Joback Method
cpg	768.59	J/mol×K	834.32	Joback Method
cpg	781.58	J/mol×K	864.25	Joback Method
cpg	793.80	J/mol×K	894.17	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=U354027&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