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

Inchi: InChI=1S/C13H22O4/c1-4-16-12(14)7-5-6-8-13(15)17-10-9-11(2)3/h2,4-10H2,1,3H3
InchiKey: CUAAYQHVUNRARX-UHFFFAOYSA-N
Formula: C13H22O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCC
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-329.97	kJ/mol	Joback Method
hf	-685.61	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.619		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	645.98	K	Joback Method
tc	827.19	K	Joback Method
tf	364.87	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.56	J/mol×K	645.98	Joback Method
cpg	560.30	J/mol×K	676.18	Joback Method
cpg	574.36	J/mol×K	706.38	Joback Method
cpg	587.74	J/mol×K	736.58	Joback Method
cpg	600.43	J/mol×K	766.79	Joback Method
cpg	612.46	J/mol×K	796.99	Joback Method
cpg	623.82	J/mol×K	827.19	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=U354024&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