Adipic acid, di(3-methylbut-3-enyl) ester

Inchi: InChI=1S/C16H26O4/c1-13(2)9-11-19-15(17)7-5-6-8-16(18)20-12-10-14(3)4/h1,3,5-12H2
InchiKey: CUSBMIUBCIBVOM-UHFFFAOYSA-N
Formula: C16H26O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCC(=C)C
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-225.42	kJ/mol	Joback Method
hf	-631.89	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	68.34	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.566		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
tb	711.18	K	Joback Method
tc	894.51	K	Joback Method
tf	382.96	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.97	J/mol×K	711.18	Joback Method
cpg	699.78	J/mol×K	741.73	Joback Method
cpg	714.77	J/mol×K	772.29	Joback Method
cpg	728.95	J/mol×K	802.84	Joback Method
cpg	742.35	J/mol×K	833.40	Joback Method
cpg	754.98	J/mol×K	863.95	Joback Method
cpg	766.86	J/mol×K	894.51	Joback Method

Sources

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=U354042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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