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

Inchi: InChI=1S/C18H32O4/c1-4-5-6-7-10-14-21-17(19)11-8-9-12-18(20)22-15-13-16(2)3/h2,4-
InchiKey: AYOLIVNMJQZZKT-UHFFFAOYSA-N
Formula: C18H32O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-287.87	kJ/mol	Joback Method
hf	-788.81	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	760.38	K	Joback Method
tc	941.30	K	Joback Method
tf	421.22	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.33	J/mol×K	760.38	Joback Method
cpg	840.31	J/mol×K	790.53	Joback Method
cpg	856.40	J/mol×K	820.69	Joback Method
cpg	871.59	J/mol×K	850.84	Joback Method
cpg	885.91	J/mol×K	880.99	Joback Method
cpg	899.38	J/mol×K	911.14	Joback Method
cpg	912.00	J/mol×K	941.30	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=U354030&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