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

Inchi: InChI=1S/C19H34O4/c1-4-5-6-7-8-11-15-22-18(20)12-9-10-13-19(21)23-16-14-17(2)3/h2
InchiKey: XZTFAMYRMAZKPY-UHFFFAOYSA-N
Formula: C19H34O4
SMILES: C=C(C)CCOC(=O)CCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-279.45	kJ/mol	Joback Method
hf	-809.45	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	75.61	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.960		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
tb	783.26	K	Joback Method
tc	965.76	K	Joback Method
tf	432.49	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.14	J/mol×K	783.26	Joback Method
cpg	899.52	J/mol×K	813.68	Joback Method
cpg	915.95	J/mol×K	844.09	Joback Method
cpg	931.43	J/mol×K	874.51	Joback Method
cpg	946.00	J/mol×K	904.93	Joback Method
cpg	959.67	J/mol×K	935.34	Joback Method
cpg	972.45	J/mol×K	965.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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