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

Inchi: InChI=1S/C23H42O4/c1-4-5-6-7-12-15-19-26-22(24)16-13-10-8-9-11-14-17-23(25)27-20
InchiKey: KAAKNVPLKCQZHO-UHFFFAOYSA-N
Formula: C23H42O4
SMILES: C=C(C)CCOC(=O)CCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-245.77	kJ/mol	Joback Method
hf	-892.01	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.520		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinpol	2654.00		NIST Webbook
rinpol	2654.00		NIST Webbook
tb	874.78	K	Joback Method
tc	1070.98	K	Joback Method
tf	477.57	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.69	J/mol×K	874.78	Joback Method
cpg	1144.76	J/mol×K	907.48	Joback Method
cpg	1162.61	J/mol×K	940.18	Joback Method
cpg	1179.25	J/mol×K	972.88	Joback Method
cpg	1194.74	J/mol×K	1005.58	Joback Method
cpg	1209.09	J/mol×K	1038.28	Joback Method
cpg	1222.35	J/mol×K	1070.98	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=U355939&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