Sebacic acid, 3-methylbut-2-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: STAHDPALDPKUHF-UHFFFAOYSA-N
Formula: C23H42O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-253.39	kJ/mol	Joback Method
hf	-900.22	kJ/mol	Joback Method
hfus	59.79	kJ/mol	Joback Method
hvap	85.14	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.520		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	931.21	kPa	Joback Method
rinpol	2685.00		NIST Webbook
tb	882.26	K	Joback Method
tc	1080.15	K	Joback Method
tf	474.25	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1127.48	J/mol×K	882.26	Joback Method
cpg	1146.53	J/mol×K	915.24	Joback Method
cpg	1164.39	J/mol×K	948.22	Joback Method
cpg	1181.09	J/mol×K	981.21	Joback Method
cpg	1196.68	J/mol×K	1014.19	Joback Method
cpg	1211.19	J/mol×K	1047.17	Joback Method
cpg	1224.66	J/mol×K	1080.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355881&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