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

Inchi: InChI=1S/C22H40O4/c1-4-5-6-11-14-18-25-21(23)15-12-9-7-8-10-13-16-22(24)26-19-17
InchiKey: STZQSQXSFGZQBJ-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: C=C(C)CCOC(=O)CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-254.19	kJ/mol	Joback Method
hf	-871.37	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.130		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	982.08	kPa	Joback Method
rinpol	2560.00		NIST Webbook
tb	851.90	K	Joback Method
tc	1043.44	K	Joback Method
tf	466.30	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.71	J/mol×K	851.90	Joback Method
cpg	1082.32	J/mol×K	883.82	Joback Method
cpg	1099.78	J/mol×K	915.75	Joback Method
cpg	1116.13	J/mol×K	947.67	Joback Method
cpg	1131.39	J/mol×K	979.59	Joback Method
cpg	1145.59	J/mol×K	1011.52	Joback Method
cpg	1158.75	J/mol×K	1043.44	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=U355938&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

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