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

Inchi: InChI=1S/C21H38O4/c1-4-5-6-13-17-24-20(22)14-11-9-7-8-10-12-15-21(23)25-18-16-19
InchiKey: KEZRJGUJLUTERV-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: C=C(C)CCOC(=O)CCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-262.61	kJ/mol	Joback Method
hf	-850.73	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.740		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1043.95	kPa	Joback Method
rinpol	2465.00		NIST Webbook
tb	829.02	K	Joback Method
tc	1016.77	K	Joback Method
tf	455.03	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.41	J/mol×K	829.02	Joback Method
cpg	1020.59	J/mol×K	860.31	Joback Method
cpg	1037.70	J/mol×K	891.60	Joback Method
cpg	1053.75	J/mol×K	922.89	Joback Method
cpg	1068.79	J/mol×K	954.19	Joback Method
cpg	1082.82	J/mol×K	985.48	Joback Method
cpg	1095.87	J/mol×K	1016.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355937&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