Sebacic acid, isohexyl 3-methylbut-2-enyl ester

Inchi: InChI=1S/C21H38O4/c1-18(2)12-11-16-24-20(22)13-9-7-5-6-8-10-14-21(23)25-17-15-19

InchiKey: VYELUPAGBKCHEF-UHFFFAOYSA-N

Formula: C21H38O4

SMILES: CC(C)=CCOC(=O)CCCCCCCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-272.67	kJ/mol	Joback Method
hf	-864.22	kJ/mol	Joback Method
hfus	51.09	kJ/mol	Joback Method
hvap	80.30	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.596		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinpol	2465.00		NIST Webbook
rinpol	2465.00		NIST Webbook
tb	836.06	K	Joback Method
tc	1026.55	K	Joback Method
tf	436.71	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.56	J/mol×K	836.06	Joback Method
cpg	1022.78	J/mol×K	867.81	Joback Method
cpg	1039.93	J/mol×K	899.56	Joback Method
cpg	1056.04	J/mol×K	931.31	Joback Method
cpg	1071.13	J/mol×K	963.06	Joback Method
cpg	1085.24	J/mol×K	994.80	Joback Method
cpg	1098.40	J/mol×K	1026.55	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=U355878&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