

Sebacic acid, isohexyl 3-methylbut-3-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:	RDKKMSDHEMAKTM-UHFFFAOYSA-N
Formula:	C21H38O4
SMILES:	<chem>C=C(C)CCOC(=O)CCCCCCCC(=O)OCCCC(C)C</chem>
Mol. weight [g/mol]:	354.52

Physical Properties

Property code	Value	Unit	Source
gf	-265.05	kJ/mol	Joback Method
hf	-856.01	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.596		Crippen Method
mvol	317.330	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	828.58	K	Joback Method
tc	1016.99	K	Joback Method
tf	440.03	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.88	J/mol×K	828.58	Joback Method
cpg	1021.13	J/mol×K	859.98	Joback Method
cpg	1038.28	J/mol×K	891.38	Joback Method
cpg	1054.36	J/mol×K	922.79	Joback Method
cpg	1069.41	J/mol×K	954.19	Joback Method
cpg	1083.43	J/mol×K	985.59	Joback Method
cpg	1096.46	J/mol×K	1016.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U355936&Units=SI

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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