

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

Inchi: InChI=1S/C24H44O4/c1-4-5-6-7-10-13-16-20-27-23(25)17-14-11-8-9-12-15-18-24(26)28
InchiKey: FTXTRPPHONRPP-UHFFFAOYSA-N
Formula: C24H44O4
SMILES: C=C(C)CCOC(=O)CCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-237.35	kJ/mol	Joback Method
hf	-912.65	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	86.74	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.910		Crippen Method
mvol	359.600	ml/mol	McGowan Method
pc	873.77	kPa	Joback Method
rinpol	2755.00		NIST Webbook
rinpol	2755.00		NIST Webbook
tb	897.66	K	Joback Method
tc	1099.45	K	Joback Method
tf	488.84	K	Joback Method
vc	1.409	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.31	J/mol×K	897.66	Joback Method
cpg	1207.87	J/mol×K	931.29	Joback Method
cpg	1226.11	J/mol×K	964.92	Joback Method
cpg	1243.07	J/mol×K	998.55	Joback Method
cpg	1258.78	J/mol×K	1032.19	Joback Method
cpg	1273.28	J/mol×K	1065.82	Joback Method
cpg	1286.62	J/mol×K	1099.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355940&Units=SI
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

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

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