

Sebacic acid, but-3-enyl nonyl ester

Inchi:	InChI=1S/C23H42O4/c1-3-5-7-8-11-14-17-21-27-23(25)19-16-13-10-9-12-15-18-22(24)2
InchiKey:	DXNXEXUFJODZPS-UHFFFAOYSA-N
Formula:	C23H42O4
SMILES:	C=CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-237.22	kJ/mol	Joback Method
hf	-882.22	kJ/mol	Joback Method
hfus	59.62	kJ/mol	Joback Method
hvap	84.43	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.520		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	922.74	kPa	Joback Method
rinqol	2662.00		NIST Webbook
tb	874.90	K	Joback Method
tc	1071.16	K	Joback Method
tf	491.53	K	Joback Method
vc	1.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.08	J/molxK	874.90	Joback Method
cpg	1145.15	J/molxK	907.61	Joback Method
cpg	1162.98	J/molxK	940.32	Joback Method
cpg	1179.62	J/molxK	973.03	Joback Method
cpg	1195.08	J/molxK	1005.74	Joback Method
cpg	1209.40	J/molxK	1038.45	Joback Method
cpg	1222.62	J/molxK	1071.16	Joback Method
dvisc	0.0006079	Paxs	491.53	Joback Method
dvisc	0.0002910	Paxs	555.42	Joback Method

dvisc	0.0001622	Paxs	619.32	Joback Method
dvisc	0.0001008	Paxs	683.22	Joback Method
dvisc	0.0000680	Paxs	747.11	Joback Method
dvisc	0.0000488	Paxs	811.01	Joback Method
dvisc	0.0000367	Paxs	874.90	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=U356089&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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