

Sebacic acid, nonyl trans-3-hexenyl ester

Inchi:	InChI=1S/C25H46O4/c1-3-5-7-9-12-15-19-23-29-25(27)21-17-14-11-10-13-16-20-24(26)
InchiKey:	NOBJOOJHIWKWGM-SOFGYWHQSA-N
Formula:	C25H46O4
SMILES:	CCC=CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	410.63

Physical Properties

Property code	Value	Unit	Source
gf	-228.00	kJ/mol	Joback Method
hf	-931.71	kJ/mol	Joback Method
hfus	66.28	kJ/mol	Joback Method
hvap	89.51	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.300		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	828.59	kPa	Joback Method
rinsol	2869.00		NIST Webbook
tb	928.14	K	Joback Method
tc	1138.56	K	Joback Method
tf	510.75	K	Joback Method
vc	1.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1253.80	J/molxK	928.14	Joback Method
cpg	1273.93	J/molxK	963.21	Joback Method
cpg	1292.67	J/molxK	998.28	Joback Method
cpg	1310.08	J/molxK	1033.35	Joback Method
cpg	1326.20	J/molxK	1068.42	Joback Method
cpg	1341.10	J/molxK	1103.49	Joback Method
cpg	1354.81	J/molxK	1138.56	Joback Method
dvisc	0.0004320	Paxs	510.75	Joback Method
dvisc	0.0001956	Paxs	580.31	Joback Method

dvisc	0.0001049	Paxs	649.88	Joback Method
dvisc	0.0000635	Paxs	719.44	Joback Method
dvisc	0.0000420	Paxs	789.01	Joback Method
dvisc	0.0000297	Paxs	858.58	Joback Method
dvisc	0.0000221	Paxs	928.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356065&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

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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