

Sebacic acid, trans-3-hexenyl propyl ester

Inchi:	InChI=1S/C19H34O4/c1-3-5-6-13-17-23-19(21)15-12-10-8-7-9-11-14-18(20)22-16-4-2/h5
InchiKey:	SKJOOCLWQWOCMV-AATRIKPKSA-N
Formula:	C19H34O4
SMILES:	CCC=CCCOC(=O)CCCCCCCCC(=O)OCCC
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-278.52	kJ/mol	Joback Method
hf	-807.87	kJ/mol	Joback Method
hfus	50.74	kJ/mol	Joback Method
hvap	76.16	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.960		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1190.70	kPa	Joback Method
rinpol	2285.00		NIST Webbook
tb	790.86	K	Joback Method
tc	974.63	K	Joback Method
tf	443.13	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.09	J/molxK	790.86	Joback Method
cpg	961.25	J/molxK	944.00	Joback Method
cpg	947.61	J/molxK	913.37	Joback Method
cpg	933.10	J/molxK	882.74	Joback Method
cpg	917.69	J/molxK	852.12	Joback Method
cpg	901.36	J/molxK	821.49	Joback Method
cpg	974.04	J/molxK	974.63	Joback Method
dvisc	0.0000533	Paxs	790.86	Joback Method
dvisc	0.0000707	Paxs	732.90	Joback Method

dvisc	0.0000983	Paxs	674.95	Joback Method
dvisc	0.0001453	Paxs	617.00	Joback Method
dvisc	0.0002331	Paxs	559.04	Joback Method
dvisc	0.0004171	Paxs	501.08	Joback Method
dvisc	0.0008689	Paxs	443.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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