

Sebacic acid, di(cis-non-3-enyl) ester

Inchi:	InChI=1S/C28H50O4/c1-3-5-7-9-13-17-21-25-31-27(29)23-19-15-11-12-16-20-24-28(30)
InchiKey:	NHRKLPJLAZTUKG-JTFWXBGUSA-N
Formula:	C28H50O4
SMILES:	CCCCC=CCCOC(=O)CCCCCCCCC(=O)OCCC=CCCCC
Mol. weight [g/mol]:	450.69

Physical Properties

Property code	Value	Unit	Source
gf	-122.52	kJ/mol	Joback Method
hf	-876.41	kJ/mol	Joback Method
hfus	74.25	kJ/mol	Joback Method
hvap	96.15	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.247		Crippen Method
mcvol	411.660	ml/mol	McGowan Method
pc	726.53	kPa	Joback Method
rinpol	3170.00		NIST Webbook
tb	1000.94	K	Joback Method
tc	1236.34	K	Joback Method
tf	539.48	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1418.29	J/molxK	1000.94	Joback Method
cpg	1439.94	J/molxK	1040.17	Joback Method
cpg	1460.04	J/molxK	1079.41	Joback Method
cpg	1478.68	J/molxK	1118.64	Joback Method
cpg	1495.98	J/molxK	1157.87	Joback Method
cpg	1512.04	J/molxK	1197.11	Joback Method
cpg	1526.96	J/molxK	1236.34	Joback Method
dvisc	0.0002721	Paxs	539.48	Joback Method
dvisc	0.0001173	Paxs	616.39	Joback Method

dvisc	0.0000610	Paxs	693.30	Joback Method
dvisc	0.0000361	Paxs	770.21	Joback Method
dvisc	0.0000235	Paxs	847.12	Joback Method
dvisc	0.0000165	Paxs	924.03	Joback Method
dvisc	0.0000122	Paxs	1000.94	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=U355931&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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