

Sebacic acid, 3-methylpentyl nonyl ester

Inchi: InChI=1S/C25H48O4/c1-4-6-7-8-11-14-17-21-28-24(26)18-15-12-9-10-13-16-19-25(27)2
InchiKey: WWDMHOMXTQJFKP-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCC(C)CC
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-310.66	kJ/mol	Joback Method
hf	-1054.21	kJ/mol	Joback Method
hfus	62.56	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.380		Crippen Method
mvol	377.990	ml/mol	McGowan Method
pc	807.99	kPa	Joback Method
rinpol	2855.00		NIST Webbook
rinpol	2855.00		NIST Webbook
tb	923.54	K	Joback Method
tc	1133.47	K	Joback Method
tf	500.83	K	Joback Method
vc	1.478	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.56	J/molxK	923.54	Joback Method
cpg	1302.20	J/molxK	958.53	Joback Method
cpg	1321.30	J/molxK	993.52	Joback Method
cpg	1338.92	J/molxK	1028.50	Joback Method
cpg	1355.09	J/molxK	1063.49	Joback Method
cpg	1369.84	J/molxK	1098.48	Joback Method
cpg	1383.23	J/molxK	1133.47	Joback Method
dvisc	0.0005334	Paxs	500.83	Joback Method

dvisc	0.0002287	Paxs	571.28	Joback Method
dvisc	0.0001181	Paxs	641.73	Joback Method
dvisc	0.0000695	Paxs	712.18	Joback Method
dvisc	0.0000450	Paxs	782.64	Joback Method
dvisc	0.0000313	Paxs	853.09	Joback Method
dvisc	0.0000230	Paxs	923.54	Joback Method

Sources

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=U355620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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