

Sebacic acid, hexyl 2-naphthyl ester

Inchi:	InChI=1S/C26H36O4/c1-2-3-4-13-20-29-25(27)16-9-7-5-6-8-10-17-26(28)30-24-19-18-22
InchiKey:	FMHXYALJEJYWLP-UHFFFAOYSA-N
Formula:	C26H36O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	412.56

Physical Properties

Property code	Value	Unit	Source
gf	-90.37	kJ/mol	Joback Method
hf	-653.44	kJ/mol	Joback Method
hfus	59.34	kJ/mol	Joback Method
hvap	96.36	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	6.989		Crippen Method
mcvol	348.860	ml/mol	McGowan Method
pc	1067.27	kPa	Joback Method
rinpol	3417.00		NIST Webbook
tb	997.50	K	Joback Method
tc	1221.46	K	Joback Method
tf	598.74	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.28	J/molxK	997.50	Joback Method
cpg	1178.20	J/molxK	1034.83	Joback Method
cpg	1192.88	J/molxK	1072.15	Joback Method
cpg	1206.39	J/molxK	1109.48	Joback Method
cpg	1218.80	J/molxK	1146.81	Joback Method
cpg	1230.19	J/molxK	1184.14	Joback Method
cpg	1240.65	J/molxK	1221.46	Joback Method
dvisc	0.0003997	Paxs	598.74	Joback Method
dvisc	0.0002351	Paxs	665.20	Joback Method

dvisc	0.0001523	Paxs	731.66	Joback Method
dvisc	0.0001061	Paxs	798.12	Joback Method
dvisc	0.0000781	Paxs	864.58	Joback Method
dvisc	0.0000601	Paxs	931.04	Joback Method
dvisc	0.0000478	Paxs	997.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354840&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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