

Sebacic acid, isobutyl 1-naphthyl ester

Inchi:	InChI=1S/C24H32O4/c1-19(2)18-27-23(25)16-7-5-3-4-6-8-17-24(26)28-22-15-11-13-20-
InchiKey:	QCSOLLVKMWWGID-UHFFFAOYSA-N
Formula:	C24H32O4
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	384.51

Physical Properties

Property code	Value	Unit	Source
gf	-109.65	kJ/mol	Joback Method
hf	-617.44	kJ/mol	Joback Method
hfus	50.64	kJ/mol	Joback Method
hvap	91.52	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.065		Crippen Method
mcvol	320.680	ml/mol	McGowan Method
pc	1221.70	kPa	Joback Method
rinpol	3114.00		NIST Webbook
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tb	951.30	K	Joback Method
tc	1169.46	K	Joback Method
tf	561.20	K	Joback Method
vc	1.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.38	J/molxK	951.30	Joback Method
cpg	1055.78	J/molxK	987.66	Joback Method
cpg	1070.00	J/molxK	1024.02	Joback Method
cpg	1083.09	J/molxK	1060.38	Joback Method
cpg	1095.11	J/molxK	1096.74	Joback Method
cpg	1106.15	J/molxK	1133.10	Joback Method
cpg	1116.25	J/molxK	1169.46	Joback Method
dvisc	0.0005292	Paxs	561.20	Joback Method

dvisc	0.0003021	Paxs	626.22	Joback Method
dvisc	0.0001917	Paxs	691.23	Joback Method
dvisc	0.0001315	Paxs	756.25	Joback Method
dvisc	0.0000958	Paxs	821.27	Joback Method
dvisc	0.0000731	Paxs	886.28	Joback Method
dvisc	0.0000578	Paxs	951.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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