Sebacic acid, isobutyl 2-naphthyl ester

Inchi: InChI=1S/C24H32O4/c1-19(2)18-27-23(25)13-7-5-3-4-6-8-14-24(26)28-22-16-15-20-11-9
InchiKey: QLBQHFWYOLFEMM-UHFFFAOYSA-N
Formula: C24H32O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc2ccccc2c1
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	3160.00		NIST Webbook
rinpol	3160.00		NIST Webbook
tb	951.30	K	Joback Method
tc	1169.46	K	Joback Method
tf	561.20	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003021	Pa×s	626.22	Joback Method
dvisc	0.0001917	Pa×s	691.23	Joback Method
dvisc	0.0001315	Pa×s	756.25	Joback Method
dvisc	0.0000958	Pa×s	821.27	Joback Method
dvisc	0.0000731	Pa×s	886.28	Joback Method
dvisc	0.0000578	Pa×s	951.30	Joback Method

Sources

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=U354836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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