Sebacic acid, isohexyl 1-naphthyl ester

Inchi: InChI=1S/C26H36O4/c1-21(2)13-12-20-29-25(27)18-7-5-3-4-6-8-19-26(28)30-24-17-11-1
InchiKey: GJXTWWYNUAWEJQ-UHFFFAOYSA-N
Formula: C26H36O4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 412.56

Physical Properties

Property code	Value	Unit	Source
gf	-92.81	kJ/mol	Joback Method
hf	-658.72	kJ/mol	Joback Method
hfus	55.82	kJ/mol	Joback Method
hvap	95.97	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	6.845		Crippen Method
mcvol	348.860	ml/mol	McGowan Method
pc	1072.87	kPa	Joback Method
rinpol	3330.00		NIST Webbook
rinpol	3330.00		NIST Webbook
tb	997.06	K	Joback Method
tc	1221.29	K	Joback Method
tf	583.74	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.62	J/mol×K	997.06	Joback Method
cpg	1178.51	J/mol×K	1034.43	Joback Method
cpg	1193.12	J/mol×K	1071.80	Joback Method
cpg	1206.54	J/mol×K	1109.17	Joback Method
cpg	1218.86	J/mol×K	1146.54	Joback Method
cpg	1230.14	J/mol×K	1183.91	Joback Method
cpg	1240.47	J/mol×K	1221.29	Joback Method
dvisc	0.0004275	Pa×s	583.74	Joback Method

dvisc	0.0002389	Pa×s	652.63	Joback Method
dvisc	0.0001492	Pa×s	721.51	Joback Method
dvisc	0.0001012	Pa×s	790.40	Joback Method
dvisc	0.0000730	Pa×s	859.29	Joback Method
dvisc	0.0000553	Pa×s	928.17	Joback Method
dvisc	0.0000435	Pa×s	997.06	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=U354808&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