Sebacic acid, heptyl 2-naphthyl ester

Inchi: InChI=1S/C27H38O4/c1-2-3-4-9-14-21-30-26(28)17-10-7-5-6-8-11-18-27(29)31-25-20-19
InchiKey: CQVYYMJAWDKGKR-UHFFFAOYSA-N
Formula: C27H38O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 426.59

Physical Properties

Property code	Value	Unit	Source
gf	-81.95	kJ/mol	Joback Method
hf	-674.08	kJ/mol	Joback Method
hfus	61.93	kJ/mol	Joback Method
hvap	98.59	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	7.380		Crippen Method
mcvol	362.950	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinpol	3524.00		NIST Webbook
rinpol	3524.00		NIST Webbook
tb	1020.38	K	Joback Method
tc	1249.29	K	Joback Method
tf	610.01	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.22	J/mol×K	1020.38	Joback Method
cpg	1293.34	J/mol×K	1211.14	Joback Method
cpg	1281.77	J/mol×K	1172.99	Joback Method
cpg	1269.16	J/mol×K	1134.83	Joback Method
cpg	1255.43	J/mol×K	1096.68	Joback Method
cpg	1240.48	J/mol×K	1058.53	Joback Method
cpg	1303.96	J/mol×K	1249.29	Joback Method
dvisc	0.0000414	Pa×s	1020.38	Joback Method

dvisc	0.0000521	Pa×s	951.98	Joback Method
dvisc	0.0000680	Pa×s	883.59	Joback Method
dvisc	0.0000928	Pa×s	815.19	Joback Method
dvisc	0.0001341	Pa×s	746.80	Joback Method
dvisc	0.0002086	Pa×s	678.40	Joback Method
dvisc	0.0003583	Pa×s	610.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354841&Units=SI

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