Sebacic acid, nonyl 2-phenoxyethyl ester

Inchi: InChI=1S/C27H44O5/c1-2-3-4-5-8-11-17-22-31-26(28)20-15-9-6-7-10-16-21-27(29)32-24
InchiKey: OUWORABDNVTAQL-UHFFFAOYSA-N
Formula: C27H44O5
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 448.64

Physical Properties

Property code	Value	Unit	Source
gf	-283.97	kJ/mol	Joback Method
hf	-985.90	kJ/mol	Joback Method
hfus	66.49	kJ/mol	Joback Method
hvap	98.69	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	7.023		Crippen Method
mcvol	388.280	ml/mol	McGowan Method
pc	863.02	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	1018.84	K	Joback Method
tc	1251.73	K	Joback Method
tf	587.02	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1336.34	J/mol×K	1018.84	Joback Method
cpg	1353.55	J/mol×K	1057.66	Joback Method
cpg	1368.89	J/mol×K	1096.47	Joback Method
cpg	1382.42	J/mol×K	1135.29	Joback Method
cpg	1394.18	J/mol×K	1174.10	Joback Method
cpg	1404.24	J/mol×K	1212.92	Joback Method
cpg	1412.65	J/mol×K	1251.73	Joback Method
dvisc	0.0002090	Pa×s	587.02	Joback Method

dvisc	0.0001041	Pa×s	658.99	Joback Method
dvisc	0.0000595	Pa×s	730.96	Joback Method
dvisc	0.0000376	Pa×s	802.93	Joback Method
dvisc	0.0000256	Pa×s	874.90	Joback Method
dvisc	0.0000185	Pa×s	946.87	Joback Method
dvisc	0.0000140	Pa×s	1018.84	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=U380787&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