Sebacic acid, phenyl tridecyl ester

Inchi: InChI=1S/C29H48O4/c1-2-3-4-5-6-7-8-9-12-15-21-26-32-28(30)24-19-13-10-11-14-20-25
InchiKey: NHSFASKMGGHWQA-UHFFFAOYSA-N
Formula: C29H48O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1
Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-162.13	kJ/mol	Joback Method
hf	-894.96	kJ/mol	Joback Method
hfus	70.48	kJ/mol	Joback Method
hvap	100.74	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	8.567		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	780.69	kPa	Joback Method
rinpol	3500.00		NIST Webbook
rinpol	3500.00		NIST Webbook
tb	1042.18	K	Joback Method
tc	1284.65	K	Joback Method
tf	587.33	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.72	J/mol×K	1042.18	Joback Method
cpg	1452.53	J/mol×K	1082.59	Joback Method
cpg	1469.48	J/mol×K	1123.00	Joback Method
cpg	1484.64	J/mol×K	1163.41	Joback Method
cpg	1498.12	J/mol×K	1203.83	Joback Method
cpg	1510.00	J/mol×K	1244.24	Joback Method
cpg	1520.37	J/mol×K	1284.65	Joback Method
dvisc	0.0002365	Pa×s	587.33	Joback Method

dvisc	0.0001126	Pa×s	663.14	Joback Method
dvisc	0.0000625	Pa×s	738.95	Joback Method
dvisc	0.0000387	Pa×s	814.75	Joback Method
dvisc	0.0000260	Pa×s	890.56	Joback Method
dvisc	0.0000186	Pa×s	966.37	Joback Method
dvisc	0.0000139	Pa×s	1042.18	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=U354517&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

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