Sebacic acid, hexyl 2-phenoxyethyl ester

Inchi: InChI=1S/C24H38O5/c1-2-3-4-14-19-28-23(25)17-12-7-5-6-8-13-18-24(26)29-21-20-27-2
InchiKey: BTXOETTXGOXBDK-UHFFFAOYSA-N
Formula: C24H38O5
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 406.56

Physical Properties

Property code	Value	Unit	Source
gf	-309.23	kJ/mol	Joback Method
hf	-923.98	kJ/mol	Joback Method
hfus	58.72	kJ/mol	Joback Method
hvap	92.02	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.853		Crippen Method
mcvol	346.010	ml/mol	McGowan Method
pc	1029.92	kPa	Joback Method
rinpol	2971.00		NIST Webbook
tb	950.20	K	Joback Method
tc	1163.33	K	Joback Method
tf	553.21	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.81	J/mol×K	950.20	Joback Method
cpg	1166.32	J/mol×K	985.72	Joback Method
cpg	1181.32	J/mol×K	1021.24	Joback Method
cpg	1194.85	J/mol×K	1056.76	Joback Method
cpg	1206.94	J/mol×K	1092.28	Joback Method
cpg	1217.62	J/mol×K	1127.80	Joback Method
cpg	1226.93	J/mol×K	1163.33	Joback Method
dvisc	0.0003049	Pa×s	553.21	Joback Method
dvisc	0.0001562	Pa×s	619.37	Joback Method

dvisc	0.0000911	Pa×s	685.54	Joback Method
dvisc	0.0000584	Pa×s	751.70	Joback Method
dvisc	0.0000402	Pa×s	817.87	Joback Method
dvisc	0.0000293	Pa×s	884.03	Joback Method
dvisc	0.0000223	Pa×s	950.20	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=U380784&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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