

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:	BTXOETTXGOXBKD-UHFFFAOYSA-N
Formula:	C24H38O5
SMILES:	CCCCCOC(=O)CCCCCCCC(=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/molxK	950.20	Joback Method
cpg	1166.32	J/molxK	985.72	Joback Method
cpg	1181.32	J/molxK	1021.24	Joback Method
cpg	1194.85	J/molxK	1056.76	Joback Method
cpg	1206.94	J/molxK	1092.28	Joback Method
cpg	1217.62	J/molxK	1127.80	Joback Method
cpg	1226.93	J/molxK	1163.33	Joback Method
dvisc	0.0003049	Paxs	553.21	Joback Method
dvisc	0.0001562	Paxs	619.37	Joback Method

dvisc	0.0000911	Paxs	685.54	Joback Method
dvisc	0.0000584	Paxs	751.70	Joback Method
dvisc	0.0000402	Paxs	817.87	Joback Method
dvisc	0.0000293	Paxs	884.03	Joback Method
dvisc	0.0000223	Paxs	950.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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