

Sebacic acid, hexyl 4-phenoxybenzyl ester

Inchi:	InChI=1S/C29H40O5/c1-2-3-4-14-23-32-28(30)17-12-7-5-6-8-13-18-29(31)33-24-25-19-2
InchiKey:	NJPRDLYGUNHTTQ-UHFFFAOYSA-N
Formula:	C29H40O5
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	468.62

Physical Properties

Property code	Value	Unit	Source
gf	-164.35	kJ/mol	Joback Method
hf	-802.12	kJ/mol	Joback Method
hfus	65.32	kJ/mol	Joback Method
hvap	106.08	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.766		Crippen Method
mvol	392.700	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	3544.00		NIST Webbook
rinpol	3544.00		NIST Webbook
tb	1096.26	K	Joback Method
tc	1344.67	K	Joback Method
tf	648.50	K	Joback Method
vc	1.510	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1348.42	J/molxK	1096.26	Joback Method
cpg	1361.96	J/molxK	1137.66	Joback Method
cpg	1373.55	J/molxK	1179.06	Joback Method
cpg	1383.24	J/molxK	1220.47	Joback Method
cpg	1391.12	J/molxK	1261.87	Joback Method
cpg	1397.26	J/molxK	1303.27	Joback Method
cpg	1401.74	J/molxK	1344.67	Joback Method
dvisc	0.0001285	Paxs	648.50	Joback Method

dvisc	0.0000689	Paxs	723.13	Joback Method
dvisc	0.0000415	Paxs	797.75	Joback Method
dvisc	0.0000273	Paxs	872.38	Joback Method
dvisc	0.0000192	Paxs	947.01	Joback Method
dvisc	0.0000142	Paxs	1021.63	Joback Method
dvisc	0.0000109	Paxs	1096.26	Joback Method

Sources

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=U355042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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