

Sebacic acid, isohexyl 4-phenoxybenzyl ester

Inchi:	InChI=1S/C29H40O5/c1-24(2)13-12-22-32-28(30)16-10-5-3-4-6-11-17-29(31)33-23-25-1
InchiKey:	MGTJTG CZNZETIS-UHFFFAOYSA-N
Formula:	C29H40O5
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	468.62

Physical Properties

Property code	Value	Unit	Source
gf	-166.79	kJ/mol	Joback Method
hf	-807.40	kJ/mol	Joback Method
hfus	61.80	kJ/mol	Joback Method
hvap	105.70	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.622		Crippen Method
mcvol	392.700	ml/mol	McGowan Method
pc	934.06	kPa	Joback Method
rinsol	3527.00		NIST Webbook
tb	1095.82	K	Joback Method
tc	1343.28	K	Joback Method
tf	633.50	K	Joback Method
vc	1.504	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1348.57	J/molxK	1095.82	Joback Method
cpg	1361.96	J/molxK	1137.06	Joback Method
cpg	1373.38	J/molxK	1178.31	Joback Method
cpg	1382.91	J/molxK	1219.55	Joback Method
cpg	1390.63	J/molxK	1260.79	Joback Method
cpg	1396.60	J/molxK	1302.03	Joback Method
cpg	1400.90	J/molxK	1343.28	Joback Method
dvisc	0.0001376	Paxs	633.50	Joback Method
dvisc	0.0000700	Paxs	710.55	Joback Method

dvisc	0.0000406	Paxs	787.61	Joback Method
dvisc	0.0000260	Paxs	864.66	Joback Method
dvisc	0.0000179	Paxs	941.71	Joback Method
dvisc	0.0000130	Paxs	1018.77	Joback Method
dvisc	0.0000099	Paxs	1095.82	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=U355041&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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