

Succinic acid, hexyl 4-phenoxybenzyl ester

Inchi:	InChI=1S/C23H28O5/c1-2-3-4-8-17-26-22(24)15-16-23(25)27-18-19-11-13-21(14-12-19)
InchiKey:	JVZILWRBLRTTQD-UHFFFAOYSA-N
Formula:	C23H28O5
SMILES:	CCCCCOC(=O)CCC(=O)OCc1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]:	384.47

Physical Properties

Property code	Value	Unit	Source
gf	-214.87	kJ/mol	Joback Method
hf	-678.28	kJ/mol	Joback Method
hfus	49.78	kJ/mol	Joback Method
hvap	92.73	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.426		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinsol	2858.00		NIST Webbook
tb	958.98	K	Joback Method
tc	1182.01	K	Joback Method
tf	580.88	K	Joback Method
vc	1.173	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.53	J/molxK	958.98	Joback Method
cpg	998.05	J/molxK	996.15	Joback Method
cpg	1010.09	J/molxK	1033.32	Joback Method
cpg	1020.69	J/molxK	1070.49	Joback Method
cpg	1029.87	J/molxK	1107.66	Joback Method
cpg	1037.67	J/molxK	1144.84	Joback Method
cpg	1044.12	J/molxK	1182.01	Joback Method
dvisc	0.0002656	Paxs	580.88	Joback Method
dvisc	0.0001511	Paxs	643.90	Joback Method

dvisc	0.0000950	Paxs	706.91	Joback Method
dvisc	0.0000644	Paxs	769.93	Joback Method
dvisc	0.0000464	Paxs	832.95	Joback Method
dvisc	0.0000349	Paxs	895.96	Joback Method
dvisc	0.0000273	Paxs	958.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349596&Units=SI
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

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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