

Phthalic acid, octyl 2-phenoxyethyl ester

Inchi:	InChI=1S/C24H30O5/c1-2-3-4-5-6-12-17-28-23(25)21-15-10-11-16-22(21)24(26)29-19-1
InchiKey:	KLVIMGRPBUFZRX-UHFFFAOYSA-N
Formula:	C24H30O5
SMILES:	CCCCCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	398.49

Physical Properties

Property code	Value	Unit	Source
gf	-206.45	kJ/mol	Joback Method
hf	-698.92	kJ/mol	Joback Method
hfus	52.37	kJ/mol	Joback Method
hvap	94.95	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.440		Crippen Method
mvol	322.250	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	3381.00		NIST Webbook
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tb	981.86	K	Joback Method
tc	1206.57	K	Joback Method
tf	592.15	K	Joback Method
vc	1.230	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.22	J/molxK	981.86	Joback Method
cpg	1096.85	J/molxK	1169.12	Joback Method
cpg	1089.24	J/molxK	1131.67	Joback Method
cpg	1080.21	J/molxK	1094.22	Joback Method
cpg	1069.72	J/molxK	1056.76	Joback Method
cpg	1057.73	J/molxK	1019.31	Joback Method
cpg	1103.08	J/molxK	1206.57	Joback Method
dvisc	0.0000236	Paxs	981.86	Joback Method

dvisc	0.0000302	Paxs	916.91	Joback Method
dvisc	0.0000402	Paxs	851.96	Joback Method
dvisc	0.0000561	Paxs	787.00	Joback Method
dvisc	0.0000832	Paxs	722.05	Joback Method
dvisc	0.0001334	Paxs	657.10	Joback Method
dvisc	0.0002370	Paxs	592.15	Joback Method

Sources

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=U382484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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