

Phthalic acid, octyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C29H32O5/c1-2-3-4-5-6-12-20-32-28(30)26-18-10-11-19-27(26)29(31)33-22-2
InchiKey:	KIOWZXIIYHIMSG-UHFFFAOYSA-N
Formula:	C29H32O5
SMILES:	CCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	460.56

Physical Properties

Property code	Value	Unit	Source
gf	-61.57	kJ/mol	Joback Method
hf	-577.06	kJ/mol	Joback Method
hfus	58.97	kJ/mol	Joback Method
hvap	109.02	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	7.353		Crippen Method
mcvol	368.940	ml/mol	McGowan Method
pc	1138.27	kPa	Joback Method
rinpol	3501.00		NIST Webbook
tb	1127.92	K	Joback Method
tc	1381.16	K	Joback Method
tf	687.44	K	Joback Method
vc	1.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1229.70	J/molxK	1127.92	Joback Method
cpg	1262.00	J/molxK	1338.96	Joback Method
cpg	1258.90	J/molxK	1296.75	Joback Method
cpg	1254.21	J/molxK	1254.54	Joback Method
cpg	1247.83	J/molxK	1212.33	Joback Method
cpg	1239.69	J/molxK	1170.13	Joback Method
cpg	1263.56	J/molxK	1381.16	Joback Method
dvisc	0.0000118	Paxs	1127.92	Joback Method
dvisc	0.0000150	Paxs	1054.51	Joback Method

dvisc	0.0000198	Paxs	981.09	Joback Method
dvisc	0.0000272	Paxs	907.68	Joback Method
dvisc	0.0000398	Paxs	834.27	Joback Method
dvisc	0.0000624	Paxs	760.85	Joback Method
dvisc	0.0001078	Paxs	687.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357039&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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