

Isophthalic acid, heptyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C28H30O5/c1-2-3-4-5-9-18-31-27(29)23-13-11-14-24(20-23)28(30)32-21-22-1
InchiKey:	MVUNCSBOESWCMV-UHFFFAOYSA-N
Formula:	C28H30O5
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OCc2cccc(Oc3ccccc3)c2)c1
Mol. weight [g/mol]:	446.53

Physical Properties

Property code	Value	Unit	Source
gf	-69.99	kJ/mol	Joback Method
hf	-556.42	kJ/mol	Joback Method
hfus	56.38	kJ/mol	Joback Method
hvap	106.80	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	6.963		Crippen Method
mcvol	354.850	ml/mol	McGowan Method
pc	1215.74	kPa	Joback Method
rinpol	3583.00		NIST Webbook
tb	1105.04	K	Joback Method
tc	1354.53	K	Joback Method
tf	676.17	K	Joback Method
vc	1.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.79	J/molxK	1105.04	Joback Method
cpg	1179.92	J/molxK	1146.62	Joback Method
cpg	1188.27	J/molxK	1188.20	Joback Method
cpg	1194.90	J/molxK	1229.79	Joback Method
cpg	1199.88	J/molxK	1271.37	Joback Method
cpg	1203.30	J/molxK	1312.95	Joback Method
cpg	1205.21	J/molxK	1354.53	Joback Method
dvisc	0.0001220	Paxs	676.17	Joback Method
dvisc	0.0000712	Paxs	747.65	Joback Method

dvisc	0.0000457	Paxs	819.13	Joback Method
dvisc	0.0000315	Paxs	890.61	Joback Method
dvisc	0.0000229	Paxs	962.08	Joback Method
dvisc	0.0000174	Paxs	1033.56	Joback Method
dvisc	0.0000137	Paxs	1105.04	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=U356610&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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