

Isophthalic acid, 3-phenoxybenzyl propyl ester

Inchi:	InChI=1S/C24H22O5/c1-2-14-27-23(25)19-9-7-10-20(16-19)24(26)28-17-18-8-6-13-22(1
InchiKey:	KOQQBQSRVYZRL-UHFFFAOYSA-N
Formula:	C24H22O5
SMILES:	CCCOC(=O)c1cccc(C(=O)OCc2cccc(Oc3ccccc3)c2)c1
Mol. weight [g/mol]:	390.43

Physical Properties

Property code	Value	Unit	Source
gf	-103.67	kJ/mol	Joback Method
hf	-473.86	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	97.89	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.403		Crippen Method
mcvol	298.490	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	3147.00		NIST Webbook
tb	1013.52	K	Joback Method
tc	1258.54	K	Joback Method
tf	631.09	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.31	J/molxK	1013.52	Joback Method
cpg	944.01	J/molxK	1054.36	Joback Method
cpg	953.06	J/molxK	1095.19	Joback Method
cpg	960.50	J/molxK	1136.03	Joback Method
cpg	966.39	J/molxK	1176.87	Joback Method
cpg	970.76	J/molxK	1217.70	Joback Method
cpg	973.68	J/molxK	1258.54	Joback Method
dvisc	0.0001945	Paxs	631.09	Joback Method
dvisc	0.0001182	Paxs	694.83	Joback Method

dvisc	0.0000781	Paxs	758.57	Joback Method
dvisc	0.0000550	Paxs	822.31	Joback Method
dvisc	0.0000408	Paxs	886.04	Joback Method
dvisc	0.0000315	Paxs	949.78	Joback Method
dvisc	0.0000251	Paxs	1013.52	Joback Method

Sources

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=U356604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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