

Isophthalic acid, isobutyl 3-phenoxybenzyl ester

Inchi:	InChI=1S/C25H24O5/c1-18(2)16-28-24(26)20-9-7-10-21(15-20)25(27)29-17-19-8-6-13-2
InchiKey:	RSVVXGKBPURNF-UHFFFAOYSA-N
Formula:	C25H24O5
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OCc2cccc(Oc3ccccc3)c2)c1
Mol. weight [g/mol]:	404.46

Physical Properties

Property code	Value	Unit	Source
gf	-97.69	kJ/mol	Joback Method
hf	-499.78	kJ/mol	Joback Method
hfus	45.09	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.649		Crippen Method
mvol	312.580	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	3197.00		NIST Webbook
tb	1035.96	K	Joback Method
tc	1282.66	K	Joback Method
tf	627.36	K	Joback Method
vc	1.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.21	J/molxK	1035.96	Joback Method
cpg	1028.38	J/molxK	1241.54	Joback Method
cpg	1024.37	J/molxK	1200.43	Joback Method
cpg	1018.80	J/molxK	1159.31	Joback Method
cpg	1011.62	J/molxK	1118.19	Joback Method
cpg	1002.77	J/molxK	1077.08	Joback Method
cpg	1030.89	J/molxK	1282.66	Joback Method
dvisc	0.0000197	Paxs	1035.96	Joback Method
dvisc	0.0000250	Paxs	967.86	Joback Method

dvisc	0.0000331	Paxs	899.76	Joback Method
dvisc	0.0000457	Paxs	831.66	Joback Method
dvisc	0.0000669	Paxs	763.56	Joback Method
dvisc	0.0001056	Paxs	695.46	Joback Method
dvisc	0.0001841	Paxs	627.36	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=U356605&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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