

Isophthalic acid, isoheyl 1-phenylpropyl ester

Inchi:	InChI=1S/C23H28O4/c1-4-21(18-11-6-5-7-12-18)27-23(25)20-14-8-13-19(16-20)22(24)2
InchiKey:	AFOPGAVZGYENMZ-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CCC(OC(=O)c1cccc(C(=O)OCCCC(C)C)c1)c1cccc1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-114.75	kJ/mol	Joback Method
hf	-556.62	kJ/mol	Joback Method
hfus	41.55	kJ/mol	Joback Method
hvap	89.54	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.588		Crippen Method
mvol	302.290	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2795.00		NIST Webbook
rinpol	2795.00		NIST Webbook
tb	935.68	K	Joback Method
tc	1161.36	K	Joback Method
tf	528.65	K	Joback Method
vc	1.143	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.93	J/molxK	935.68	Joback Method
cpg	972.48	J/molxK	973.29	Joback Method
cpg	985.61	J/molxK	1010.91	Joback Method
cpg	997.36	J/molxK	1048.52	Joback Method
cpg	1007.80	J/molxK	1086.13	Joback Method
cpg	1016.97	J/molxK	1123.75	Joback Method
cpg	1024.91	J/molxK	1161.36	Joback Method
dvisc	0.0004639	Paxs	528.65	Joback Method

dvisc	0.0002279	Paxs	596.49	Joback Method
dvisc	0.0001294	Paxs	664.33	Joback Method
dvisc	0.0000816	Paxs	732.17	Joback Method
dvisc	0.0000557	Paxs	800.00	Joback Method
dvisc	0.0000403	Paxs	867.84	Joback Method
dvisc	0.0000306	Paxs	935.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344551&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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