

Isophthalic acid, 1-naphthyl pentyl ester

Inchi:	InChI=1S/C23H22O4/c1-2-3-6-15-26-22(24)18-11-7-12-19(16-18)23(25)27-21-14-8-10-1
InchiKey:	SXQMDNHLLUOILA-UHFFFAOYSA-N
Formula:	C23H22O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)O)c2cccc3ccccc23)c1
Mol. weight [g/mol]:	362.42

Physical Properties

Property code	Value	Unit	Source
gf	-12.85	kJ/mol	Joback Method
hf	-366.46	kJ/mol	Joback Method
hfus	45.22	kJ/mol	Joback Method
hvap	92.62	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	5.406		Crippen Method
mvol	282.830	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	3187.00		NIST Webbook
rinpol	3187.00		NIST Webbook
tb	960.52	K	Joback Method
tc	1197.59	K	Joback Method
tf	603.87	K	Joback Method
vc	1.077	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.15	J/molxK	960.52	Joback Method
cpg	887.05	J/molxK	1000.03	Joback Method
cpg	898.77	J/molxK	1039.54	Joback Method
cpg	909.37	J/molxK	1079.06	Joback Method
cpg	918.94	J/molxK	1118.57	Joback Method
cpg	927.56	J/molxK	1158.08	Joback Method
cpg	935.31	J/molxK	1197.59	Joback Method
dvisc	0.0004574	Paxs	603.87	Joback Method

dvisc	0.0002984	Paxs	663.31	Joback Method
dvisc	0.0002088	Paxs	722.75	Joback Method
dvisc	0.0001542	Paxs	782.19	Joback Method
dvisc	0.0001189	Paxs	841.64	Joback Method
dvisc	0.0000949	Paxs	901.08	Joback Method
dvisc	0.0000779	Paxs	960.52	Joback Method

Sources

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=U344688&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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