

Isophthalic acid, hexyl 2-methoxyethyl ester

Inchi:	InChI=1S/C17H24O5/c1-3-4-5-6-10-21-16(18)14-8-7-9-15(13-14)17(19)22-12-11-20-2/h
InchiKey:	BOPNIVKUAYXNKO-UHFFFAOYSA-N
Formula:	C17H24O5
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OCCOC)c1
Mol. weight [g/mol]:	308.37

Physical Properties

Property code	Value	Unit	Source
gf	-377.80	kJ/mol	Joback Method
hf	-790.97	kJ/mol	Joback Method
hfus	40.20	kJ/mol	Joback Method
hvap	77.10	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.227		Crippen Method
mvol	247.380	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2333.00		NIST Webbook
rinpol	2333.00		NIST Webbook
tb	795.02	K	Joback Method
tc	995.27	K	Joback Method
tf	486.84	K	Joback Method
vc	0.946	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.69	J/molxK	795.02	Joback Method
cpg	747.70	J/molxK	828.40	Joback Method
cpg	761.66	J/molxK	861.77	Joback Method
cpg	774.58	J/molxK	895.15	Joback Method
cpg	786.44	J/molxK	928.52	Joback Method
cpg	797.27	J/molxK	961.90	Joback Method
cpg	807.05	J/molxK	995.27	Joback Method
dvisc	0.0005581	Paxs	486.84	Joback Method

dvisc	0.0003254	Paxs	538.20	Joback Method
dvisc	0.0002084	Paxs	589.57	Joback Method
dvisc	0.0001434	Paxs	640.93	Joback Method
dvisc	0.0001043	Paxs	692.29	Joback Method
dvisc	0.0000792	Paxs	743.66	Joback Method
dvisc	0.0000624	Paxs	795.02	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=U345861&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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