

Isophthalic acid, 2-ethoxyethyl octyl ester

Inchi:	InChI=1S/C20H30O5/c1-3-5-6-7-8-9-13-24-19(21)17-11-10-12-18(16-17)20(22)25-15-14
InchiKey:	LLPCCAQWIPZIFF-UHFFFAOYSA-N
Formula:	C20H30O5
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OCCOCC)c1
Mol. weight [g/mol]:	350.45

Physical Properties

Property code	Value	Unit	Source
gf	-352.54	kJ/mol	Joback Method
hf	-852.89	kJ/mol	Joback Method
hfus	47.97	kJ/mol	Joback Method
hvap	83.77	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.397		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2601.00		NIST Webbook
rinpol	2601.00		NIST Webbook
tb	863.66	K	Joback Method
tc	1065.19	K	Joback Method
tf	520.65	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.10	J/molxK	863.66	Joback Method
cpg	973.30	J/molxK	1031.61	Joback Method
cpg	962.45	J/molxK	998.02	Joback Method
cpg	950.41	J/molxK	964.43	Joback Method
cpg	937.18	J/molxK	930.84	Joback Method
cpg	922.75	J/molxK	897.25	Joback Method
cpg	982.99	J/molxK	1065.19	Joback Method
dvisc	0.0000411	Paxs	863.66	Joback Method

dvisc	0.0000527	Paxs	806.49	Joback Method
dvisc	0.0000703	Paxs	749.32	Joback Method
dvisc	0.0000982	Paxs	692.15	Joback Method
dvisc	0.0001457	Paxs	634.99	Joback Method
dvisc	0.0002338	Paxs	577.82	Joback Method
dvisc	0.0004161	Paxs	520.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345851&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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