

Isophthalic acid, 2-ethoxyethyl nonyl ester

Inchi:	InChI=1S/C21H32O5/c1-3-5-6-7-8-9-10-14-25-20(22)18-12-11-13-19(17-18)21(23)26-16
InchiKey:	HQBDHOLPQDGYAZ-UHFFFAOYSA-N
Formula:	C21H32O5
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCCOCC)c1
Mol. weight [g/mol]:	364.48

Physical Properties

Property code	Value	Unit	Source
gf	-344.12	kJ/mol	Joback Method
hf	-873.53	kJ/mol	Joback Method
hfus	50.56	kJ/mol	Joback Method
hvap	86.00	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.787		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2704.00		NIST Webbook
rinpol	2704.00		NIST Webbook
tb	886.54	K	Joback Method
tc	1089.96	K	Joback Method
tf	531.92	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.74	J/molxK	886.54	Joback Method
cpg	1033.23	J/molxK	1056.05	Joback Method
cpg	1022.43	J/molxK	1022.15	Joback Method
cpg	1010.40	J/molxK	988.25	Joback Method
cpg	997.11	J/molxK	954.35	Joback Method
cpg	982.57	J/molxK	920.44	Joback Method
cpg	1042.80	J/molxK	1089.96	Joback Method
dvisc	0.0000356	Paxs	886.54	Joback Method

dvisc	0.0000458	Paxs	827.44	Joback Method
dvisc	0.0000612	Paxs	768.33	Joback Method
dvisc	0.0000860	Paxs	709.23	Joback Method
dvisc	0.0001284	Paxs	650.13	Joback Method
dvisc	0.0002078	Paxs	591.02	Joback Method
dvisc	0.0003742	Paxs	531.92	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=U345852&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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