

Isophthalic acid, 2-ethoxyethyl heptyl ester

Inchi:	InChI=1S/C19H28O5/c1-3-5-6-7-8-12-23-18(20)16-10-9-11-17(15-16)19(21)24-14-13-22
InchiKey:	PJGAATLUVMTYQW-UHFFFAOYSA-N
Formula:	C19H28O5
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OCCOCC)c1
Mol. weight [g/mol]:	336.42

Physical Properties

Property code	Value	Unit	Source
gf	-360.96	kJ/mol	Joback Method
hf	-832.25	kJ/mol	Joback Method
hfus	45.38	kJ/mol	Joback Method
hvap	81.55	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.007		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	2497.00		NIST Webbook
tb	840.78	K	Joback Method
tc	1041.20	K	Joback Method
tf	509.38	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.17	J/molxK	840.78	Joback Method
cpg	863.62	J/molxK	874.18	Joback Method
cpg	877.92	J/molxK	907.59	Joback Method
cpg	891.07	J/molxK	940.99	Joback Method
cpg	903.09	J/molxK	974.39	Joback Method
cpg	913.97	J/molxK	1007.79	Joback Method
cpg	923.73	J/molxK	1041.20	Joback Method
dvisc	0.0004609	Paxs	509.38	Joback Method
dvisc	0.0002620	Paxs	564.61	Joback Method

dvisc	0.0001648	Paxs	619.85	Joback Method
dvisc	0.0001118	Paxs	675.08	Joback Method
dvisc	0.0000804	Paxs	730.31	Joback Method
dvisc	0.0000606	Paxs	785.55	Joback Method
dvisc	0.0000474	Paxs	840.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345850&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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