

Isophthalic acid, ethyl 2-methylbutyl ester

Inchi:	InChI=1S/C15H20O4/c1-4-11(3)10-19-15(17)13-8-6-7-12(9-13)14(16)18-5-2/h6-9,11H,4-
InchiKey:	CQBQQCIIHPLINM-UHFFFAOYSA-N
Formula:	C15H20O4
SMILES:	CCOC(=O)c1cccc(C(=O)OCC(C)CC)c1
Mol. weight [g/mol]:	264.32

Physical Properties

Property code	Value	Unit	Source
gf	-292.08	kJ/mol	Joback Method
hf	-622.75	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	69.85	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.066		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	726.40	K	Joback Method
tc	933.26	K	Joback Method
tf	427.07	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.17	J/molxK	726.40	Joback Method
cpg	609.21	J/molxK	760.88	Joback Method
cpg	623.26	J/molxK	795.35	Joback Method
cpg	636.36	J/molxK	829.83	Joback Method
cpg	648.50	J/molxK	864.30	Joback Method
cpg	659.69	J/molxK	898.78	Joback Method
cpg	669.96	J/molxK	933.26	Joback Method
dvisc	0.0010677	Paxs	427.07	Joback Method

dvisc	0.0005817	Paxs	476.96	Joback Method
dvisc	0.0003556	Paxs	526.85	Joback Method
dvisc	0.0002367	Paxs	576.74	Joback Method
dvisc	0.0001681	Paxs	626.62	Joback Method
dvisc	0.0001255	Paxs	676.51	Joback Method
dvisc	0.0000976	Paxs	726.40	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=U344727&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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