

Isophthalic acid, 2-methoxyethyl isobutyl ester

Inchi:	InChI=1S/C15H20O5/c1-11(2)10-20-15(17)13-6-4-5-12(9-13)14(16)19-8-7-18-3/h4-6,9,1
InchiKey:	RPHCKIKSGYJDJM-UHFFFAOYSA-N
Formula:	C15H20O5
SMILES:	COCCOC(=O)c1cccc(C(=O)OCC(C)C)c1
Mol. weight [g/mol]:	280.32

Physical Properties

Property code	Value	Unit	Source
gf	-397.08	kJ/mol	Joback Method
hf	-754.97	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	72.26	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.303		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	748.82	K	Joback Method
tc	954.33	K	Joback Method
tf	449.30	K	Joback Method
vc	0.828	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.47	J/molxK	748.82	Joback Method
cpg	636.13	J/molxK	783.07	Joback Method
cpg	649.79	J/molxK	817.32	Joback Method
cpg	662.46	J/molxK	851.57	Joback Method
cpg	674.12	J/molxK	885.82	Joback Method
cpg	684.78	J/molxK	920.08	Joback Method
cpg	694.42	J/molxK	954.33	Joback Method
dvisc	0.0007579	Paxs	449.30	Joback Method

dvisc	0.0004248	Paxs	499.22	Joback Method
dvisc	0.0002645	Paxs	549.14	Joback Method
dvisc	0.0001782	Paxs	599.06	Joback Method
dvisc	0.0001276	Paxs	648.98	Joback Method
dvisc	0.0000958	Paxs	698.90	Joback Method
dvisc	0.0000748	Paxs	748.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345858&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

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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