

Isophthalic acid, 3-methylbut-2-yl propyl ester

Inchi:	InChI=1S/C16H22O4/c1-5-9-19-15(17)13-7-6-8-14(10-13)16(18)20-12(4)11(2)3/h6-8,10-
InchiKey:	NBSJJCMQBWSTJY-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	CCCOC(=O)c1cccc(C(=O)OC(C)C(C)C)c1
Mol. weight [g/mol]:	278.34

Physical Properties

Property code	Value	Unit	Source
gf	-286.10	kJ/mol	Joback Method
hf	-648.67	kJ/mol	Joback Method
hfus	29.38	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.455		Crippen Method
mvol	227.420	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	2015.00		NIST Webbook
tb	748.84	K	Joback Method
tc	956.66	K	Joback Method
tf	423.34	K	Joback Method
vc	0.860	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.54	J/molxK	748.84	Joback Method
cpg	665.13	J/molxK	783.48	Joback Method
cpg	679.68	J/molxK	818.11	Joback Method
cpg	693.19	J/molxK	852.75	Joback Method
cpg	705.67	J/molxK	887.39	Joback Method
cpg	717.14	J/molxK	922.02	Joback Method
cpg	727.62	J/molxK	956.66	Joback Method
dvisc	0.0011585	Paxs	423.34	Joback Method
dvisc	0.0005749	Paxs	477.59	Joback Method

dvisc	0.0003291	Paxs	531.84	Joback Method
dvisc	0.0002089	Paxs	586.09	Joback Method
dvisc	0.0001432	Paxs	640.34	Joback Method
dvisc	0.0001042	Paxs	694.59	Joback Method
dvisc	0.0000793	Paxs	748.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344718&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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