

Phthalic acid, isobutyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C20H30O4/c1-14(2)12-23-18(21)16-9-7-8-10-17(16)19(22)24-13-15(3)11-20(4)
InchiKey:	XRCKQJJXYYV NKZ-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CC(C)COC(=O)c1cccc1C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-249.58	kJ/mol	Joback Method
hf	-739.98	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	79.29	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.729		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	837.13	K	Joback Method
tc	1046.77	K	Joback Method
tf	470.84	K	Joback Method
vc	1.073	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.79	J/molxK	837.13	Joback Method
cpg	896.41	J/molxK	872.07	Joback Method
cpg	911.81	J/molxK	907.01	Joback Method
cpg	926.03	J/molxK	941.95	Joback Method
cpg	939.11	J/molxK	976.89	Joback Method
cpg	951.11	J/molxK	1011.83	Joback Method
cpg	962.05	J/molxK	1046.77	Joback Method
dvisc	0.0007329	Paxs	470.84	Joback Method

dvisc	0.0003336	Paxs	531.89	Joback Method
dvisc	0.0001786	Paxs	592.94	Joback Method
dvisc	0.0001074	Paxs	653.99	Joback Method
dvisc	0.0000705	Paxs	715.03	Joback Method
dvisc	0.0000494	Paxs	776.08	Joback Method
dvisc	0.0000365	Paxs	837.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377769&Units=SI

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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