

Isophthalic acid, 2-methylcyclohexyl propyl ester

Inchi:	InChI=1S/C18H24O4/c1-3-11-21-17(19)14-8-6-9-15(12-14)18(20)22-16-10-5-4-7-13(16)2
InchiKey:	ZVNYDPRPVKVKDG-UHFFFAOYSA-N
Formula:	C18H24O4
SMILES:	CCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1
Mol. weight [g/mol]:	304.38

Physical Properties

Property code	Value	Unit	Source
gf	-247.64	kJ/mol	Joback Method
hf	-645.41	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	77.03	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.989		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	810.36	K	Joback Method
tc	1033.61	K	Joback Method
tf	479.02	K	Joback Method
vc	0.915	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.48	J/molxK	810.36	Joback Method
cpg	832.13	J/molxK	996.40	Joback Method
cpg	820.52	J/molxK	959.19	Joback Method
cpg	807.47	J/molxK	921.99	Joback Method
cpg	792.95	J/molxK	884.78	Joback Method
cpg	776.97	J/molxK	847.57	Joback Method
cpg	842.31	J/molxK	1033.61	Joback Method
dvisc	0.0000955	Paxs	810.36	Joback Method

dvisc	0.0001207	Paxs	755.14	Joback Method
dvisc	0.0001584	Paxs	699.91	Joback Method
dvisc	0.0002178	Paxs	644.69	Joback Method
dvisc	0.0003179	Paxs	589.47	Joback Method
dvisc	0.0005015	Paxs	534.24	Joback Method
dvisc	0.0008791	Paxs	479.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345746&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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