

Isophthalic acid, cyclohexylmethyl propyl ester

Inchi:	InChI=1S/C18H24O4/c1-2-11-21-17(19)15-9-6-10-16(12-15)18(20)22-13-14-7-4-3-5-8-14
InchiKey:	TZZRPBFNJJPQCN-UHFFFAOYSA-N
Formula:	C18H24O4
SMILES:	CCCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]:	304.38

Physical Properties

Property code	Value	Unit	Source
gf	-239.93	kJ/mol	Joback Method
hf	-625.07	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	77.34	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.990		Crippen Method
mvol	244.740	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	815.03	K	Joback Method
tc	1038.33	K	Joback Method
tf	483.26	K	Joback Method
vc	0.916	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.87	J/molxK	815.03	Joback Method
cpg	772.90	J/molxK	852.25	Joback Method
cpg	788.49	J/molxK	889.46	Joback Method
cpg	802.66	J/molxK	926.68	Joback Method
cpg	815.43	J/molxK	963.90	Joback Method
cpg	826.83	J/molxK	1001.11	Joback Method
cpg	836.90	J/molxK	1038.33	Joback Method
dvisc	0.0008245	Paxs	483.26	Joback Method

dvisc	0.0004502	Paxs	538.55	Joback Method
dvisc	0.0002751	Paxs	593.85	Joback Method
dvisc	0.0001828	Paxs	649.14	Joback Method
dvisc	0.0001296	Paxs	704.44	Joback Method
dvisc	0.0000965	Paxs	759.73	Joback Method
dvisc	0.0000749	Paxs	815.03	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=U343824&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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