

Isophthalic acid, cyclohexylmethyl ethyl ester

Inchi:	InChI=1S/C17H22O4/c1-2-20-16(18)14-9-6-10-15(11-14)17(19)21-12-13-7-4-3-5-8-13/h6
InchiKey:	KBWMCBYGRYSMDX-UHFFFAOYSA-N
Formula:	C17H22O4
SMILES:	CCOC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]:	290.35

Physical Properties

Property code	Value	Unit	Source
gf	-248.35	kJ/mol	Joback Method
hf	-604.43	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	75.12	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.600		Crippen Method
mvol	230.650	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2326.00		NIST Webbook
rinpol	2326.00		NIST Webbook
tb	792.15	K	Joback Method
tc	1018.40	K	Joback Method
tf	471.99	K	Joback Method
vc	0.861	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.54	J/molxK	792.15	Joback Method
cpg	769.58	J/molxK	980.69	Joback Method
cpg	758.14	J/molxK	942.98	Joback Method
cpg	745.34	J/molxK	905.27	Joback Method
cpg	731.16	J/molxK	867.57	Joback Method
cpg	715.57	J/molxK	829.86	Joback Method
cpg	779.69	J/molxK	1018.40	Joback Method
dvisc	0.0000856	Paxs	792.15	Joback Method

dvisc	0.0001100	Paxs	738.79	Joback Method
dvisc	0.0001470	Paxs	685.43	Joback Method
dvisc	0.0002064	Paxs	632.07	Joback Method
dvisc	0.0003085	Paxs	578.71	Joback Method
dvisc	0.0005003	Paxs	525.35	Joback Method
dvisc	0.0009049	Paxs	471.99	Joback Method

Sources

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=U343823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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