

Isophthalic acid, cyclohexylmethyl isobutyl ester

Inchi:	InChI=1S/C19H26O4/c1-14(2)12-22-18(20)16-9-6-10-17(11-16)19(21)23-13-15-7-4-3-5-8
InchiKey:	VPQCZLNBAOBINH-UHFFFAOYSA-N
Formula:	C19H26O4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]:	318.41

Physical Properties

Property code	Value	Unit	Source
gf	-233.95	kJ/mol	Joback Method
hf	-650.99	kJ/mol	Joback Method
hfus	32.50	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.237		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	2490.00		NIST Webbook
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tb	837.47	K	Joback Method
tc	1061.50	K	Joback Method
tf	479.53	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.54	J/molxK	837.47	Joback Method
cpg	831.77	J/molxK	874.81	Joback Method
cpg	847.48	J/molxK	912.15	Joback Method
cpg	861.71	J/molxK	949.48	Joback Method
cpg	874.48	J/molxK	986.82	Joback Method
cpg	885.82	J/molxK	1024.16	Joback Method
cpg	895.76	J/molxK	1061.50	Joback Method
dvisc	0.0008523	Paxs	479.53	Joback Method

dvisc	0.0004285	Paxs	539.19	Joback Method
dvisc	0.0002471	Paxs	598.84	Joback Method
dvisc	0.0001574	Paxs	658.50	Joback Method
dvisc	0.0001081	Paxs	718.16	Joback Method
dvisc	0.0000786	Paxs	777.81	Joback Method
dvisc	0.0000598	Paxs	837.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343825&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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