

Isophthalic acid, dicyclohexylmethyl ester

Inchi:	InChI=1S/C22H30O4/c23-21(25-15-17-8-3-1-4-9-17)19-12-7-13-20(14-19)22(24)26-16-1
InchiKey:	BIMUWGJXLYCZOP-UHFFFAOYSA-N
Formula:	C22H30O4
SMILES:	O=C(OCC1CCCCC1)c1cccc(C(=O)OCC2CCCCC2)c1
Mol. weight [g/mol]:	358.47

Physical Properties

Property code	Value	Unit	Source
gf	-181.80	kJ/mol	Joback Method
hf	-653.31	kJ/mol	Joback Method
hfus	35.63	kJ/mol	Joback Method
hvap	86.67	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.161		Crippen Method
mvol	290.240	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	3014.00		NIST Webbook
rinpol	3014.00		NIST Webbook
tb	926.10	K	Joback Method
tc	1165.62	K	Joback Method
tf	535.72	K	Joback Method
vc	1.073	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.52	J/molxK	926.10	Joback Method
cpg	1004.81	J/molxK	966.02	Joback Method
cpg	1020.10	J/molxK	1005.94	Joback Method
cpg	1033.46	J/molxK	1045.86	Joback Method
cpg	1044.92	J/molxK	1085.78	Joback Method
cpg	1054.56	J/molxK	1125.70	Joback Method
cpg	1062.41	J/molxK	1165.62	Joback Method
dvisc	0.0006111	Paxs	535.72	Joback Method

dvisc	0.0003105	Paxs	600.78	Joback Method
dvisc	0.0001801	Paxs	665.85	Joback Method
dvisc	0.0001151	Paxs	730.91	Joback Method
dvisc	0.0000791	Paxs	795.97	Joback Method
dvisc	0.0000576	Paxs	861.04	Joback Method
dvisc	0.0000438	Paxs	926.10	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=U343835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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