

Isophthalic acid, cyclohexylmethyl hexyl ester

Inchi:	InChI=1S/C21H30O4/c1-2-3-4-8-14-24-20(22)18-12-9-13-19(15-18)21(23)25-16-17-10-6
InchiKey:	FOSHKIVRCKVXKF-UHFFFAOYSA-N
Formula:	C21H30O4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OCC2CCCC2)c1
Mol. weight [g/mol]:	346.46

Physical Properties

Property code	Value	Unit	Source
gf	-214.67	kJ/mol	Joback Method
hf	-686.99	kJ/mol	Joback Method
hfus	41.21	kJ/mol	Joback Method
hvap	84.02	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.161		Crippen Method
mvol	287.010	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	2754.00		NIST Webbook
rinpol	2754.00		NIST Webbook
tb	883.67	K	Joback Method
tc	1101.87	K	Joback Method
tf	517.07	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.47	J/molxK	883.67	Joback Method
cpg	949.38	J/molxK	920.04	Joback Method
cpg	964.77	J/molxK	956.40	Joback Method
cpg	978.69	J/molxK	992.77	Joback Method
cpg	991.18	J/molxK	1029.14	Joback Method
cpg	1002.26	J/molxK	1065.51	Joback Method
cpg	1011.97	J/molxK	1101.87	Joback Method
dvisc	0.0006068	Paxs	517.07	Joback Method

dvisc	0.0003200	Paxs	578.17	Joback Method
dvisc	0.0001907	Paxs	639.27	Joback Method
dvisc	0.0001244	Paxs	700.37	Joback Method
dvisc	0.0000869	Paxs	761.47	Joback Method
dvisc	0.0000640	Paxs	822.57	Joback Method
dvisc	0.0000492	Paxs	883.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343829&Units=SI

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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