

Cyclohexyl isooctyl phthalate

Inchi:	InChI=1S/C22H32O4/c1-17(2)11-5-4-10-16-25-21(23)19-14-8-9-15-20(19)22(24)26-18-1
InchiKey:	PQDNDGYLGVVELW-UHFFFAOYSA-N
Formula:	C22H32O4
SMILES:	CC(C)CCCCOC(=O)c1cccc1C(=O)OC1CCCCC1
Mol. weight [g/mol]:	360.49
CAS:	71486-48-1

Physical Properties

Property code	Value	Unit	Source
gf	-208.69	kJ/mol	Joback Method
hf	-712.91	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	85.86	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.549		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2446.00		NIST Webbook
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rinpol	2446.00		NIST Webbook
tb	906.11	K	Joback Method
tc	1126.08	K	Joback Method
tf	513.34	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.13	J/molxK	906.11	Joback Method
cpg	1010.08	J/molxK	942.77	Joback Method
cpg	1025.46	J/molxK	979.43	Joback Method
cpg	1039.30	J/molxK	1016.09	Joback Method
cpg	1051.65	J/molxK	1052.75	Joback Method
cpg	1062.53	J/molxK	1089.41	Joback Method

cpg	1071.99	J/mol×K	1126.08	Joback Method
dvisc	0.0006115	Paxs	513.34	Joback Method
dvisc	0.0002980	Paxs	578.80	Joback Method
dvisc	0.0001681	Paxs	644.26	Joback Method
dvisc	0.0001053	Paxs	709.72	Joback Method
dvisc	0.0000714	Paxs	775.19	Joback Method
dvisc	0.0000515	Paxs	840.65	Joback Method
dvisc	0.0000389	Paxs	906.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71486481&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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