

Isophthalic acid, 6-chlorohexyl ethyl ester

Inchi:	InChI=1S/C16H21ClO4/c1-2-20-15(18)13-8-7-9-14(12-13)16(19)21-11-6-4-3-5-10-17/h7-
InchiKey:	CUVFBJQPUVIWQR-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	CCOC(=O)c1cccc(C(=O)OCCCCCl)c1
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-293.15	kJ/mol	Joback Method
hf	-653.85	kJ/mol	Joback Method
hfus	40.62	kJ/mol	Joback Method
hvap	76.85	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.819		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	787.15	K	Joback Method
tc	992.74	K	Joback Method
tf	483.26	K	Joback Method
vc	0.920	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.20	J/molxK	787.15	Joback Method
cpg	689.21	J/molxK	821.42	Joback Method
cpg	702.22	J/molxK	855.68	Joback Method
cpg	714.27	J/molxK	889.95	Joback Method
cpg	725.35	J/molxK	924.21	Joback Method
cpg	735.49	J/molxK	958.48	Joback Method
cpg	744.69	J/molxK	992.74	Joback Method
dvisc	0.0007196	Paxs	483.26	Joback Method

dvisc	0.0004230	Paxs	533.91	Joback Method
dvisc	0.0002726	Paxs	584.56	Joback Method
dvisc	0.0001884	Paxs	635.21	Joback Method
dvisc	0.0001376	Paxs	685.85	Joback Method
dvisc	0.0001049	Paxs	736.50	Joback Method
dvisc	0.0000828	Paxs	787.15	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=U345876&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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