

Terephthalic acid, 4-chloro-2-methylbenzyl hexyl ester

Inchi:	InChI=1S/C22H25ClO4/c1-3-4-5-6-13-26-21(24)17-7-9-18(10-8-17)22(25)27-15-19-11-12
InchiKey:	KFPBWZGRLHLOJI-UHFFFAOYSA-N
Formula:	C22H25ClO4
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCc2ccc(Cl)cc2C)cc1
Mol. weight [g/mol]:	388.88

Physical Properties

Property code	Value	Unit	Source
gf	-149.48	kJ/mol	Joback Method
hf	-564.10	kJ/mol	Joback Method
hfus	49.42	kJ/mol	Joback Method
hvap	93.80	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	5.743		Crippen Method
mvol	300.440	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	3178.00		NIST Webbook
tb	961.07	K	Joback Method
tc	1188.91	K	Joback Method
tf	602.34	K	Joback Method
vc	1.149	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.44	J/molxK	961.07	Joback Method
cpg	931.16	J/molxK	999.04	Joback Method
cpg	942.53	J/molxK	1037.02	Joback Method
cpg	952.57	J/molxK	1074.99	Joback Method
cpg	961.32	J/molxK	1112.96	Joback Method
cpg	968.82	J/molxK	1150.94	Joback Method
cpg	975.10	J/molxK	1188.91	Joback Method
dvisc	0.0002765	Paxs	602.34	Joback Method
dvisc	0.0001711	Paxs	662.13	Joback Method

dvisc	0.0001146	Paxs	721.92	Joback Method
dvisc	0.0000816	Paxs	781.71	Joback Method
dvisc	0.0000610	Paxs	841.49	Joback Method
dvisc	0.0000474	Paxs	901.28	Joback Method
dvisc	0.0000380	Paxs	961.07	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=U416111&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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