

2-[(Trichloroacetyl)oxy][1,1'-biphenyl]-3-carboxylic acid

Inchi:
InchiKey:

InChI=1S/C15H9Cl3O4/c16-15(17,18)14(21)22-12-10(9-5-2-1-3-6-9)7-4-8-11(12)13(19)2

XQPICHPIPPJBOD-UHFFFAOYSA-N

Formula:

C15H9Cl3O4

SMILES:

O=C(O)c1cccc(-c2ccccc2)c1OC(=O)C(Cl)(Cl)Cl

Mol. weight [g/mol]:

359.59

CAS:

116401-04-8

Physical Properties

Property code	Value	Unit	Source
gf	-251.63	kJ/mol	Joback Method
hf	-468.39	kJ/mol	Joback Method
hfus	35.56	kJ/mol	Joback Method
hvap	99.30	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.327		Crippen Method
mcvol	226.290	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	937.32	K	Joback Method
tc	1182.13	K	Joback Method
tf	611.78	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.91	J/molxK	937.32	Joback Method
cpg	588.05	J/molxK	978.12	Joback Method
cpg	594.40	J/molxK	1018.92	Joback Method
cpg	600.05	J/molxK	1059.73	Joback Method
cpg	605.08	J/molxK	1100.53	Joback Method
cpg	609.58	J/molxK	1141.33	Joback Method
cpg	613.62	J/molxK	1182.13	Joback Method
dvisc	0.0001574	Paxs	611.78	Joback Method
dvisc	0.0000833	Paxs	666.04	Joback Method

dvisc	0.0000486	Paxs	720.29	Joback Method
dvisc	0.0000305	Paxs	774.55	Joback Method
dvisc	0.0000204	Paxs	828.81	Joback Method
dvisc	0.0000143	Paxs	883.06	Joback Method
dvisc	0.0000105	Paxs	937.32	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=C116401048&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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