

2,6-Bis(chloromethyl)-p-tolyl acetate

Inchi:	InChI=1S/C11H12Cl2O2/c1-7-3-9(5-12)11(15-8(2)14)10(4-7)6-13/h3-4H,5-6H2,1-2H3
InchiKey:	KUMMZJSZVNWQLZ-UHFFFAOYSA-N
Formula:	C11H12Cl2O2
SMILES:	CC(=O)Oc1c(CCl)cc(C)cc1CCl
Mol. weight [g/mol]:	247.12
CAS:	19228-70-7

Physical Properties

Property code	Value	Unit	Source
gf	-132.52	kJ/mol	Joback Method
hf	-344.53	kJ/mol	Joback Method
hfus	28.30	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.398		Crippen Method
mcvol	174.010	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	643.85	K	Joback Method
tc	863.69	K	Joback Method
tf	409.71	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.81	J/molxK	643.85	Joback Method
cpg	448.86	J/molxK	827.05	Joback Method
cpg	439.64	J/molxK	790.41	Joback Method
cpg	429.74	J/molxK	753.77	Joback Method
cpg	419.13	J/molxK	717.13	Joback Method
cpg	407.83	J/molxK	680.49	Joback Method
cpg	457.39	J/molxK	863.69	Joback Method
dvisc	0.0001769	Paxs	643.85	Joback Method
dvisc	0.0002148	Paxs	604.83	Joback Method

dvisc	0.0002678	Paxs	565.80	Joback Method
dvisc	0.0003452	Paxs	526.78	Joback Method
dvisc	0.0004632	Paxs	487.76	Joback Method
dvisc	0.0006542	Paxs	448.73	Joback Method
dvisc	0.0009869	Paxs	409.71	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=C19228707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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