2,4-Dichlorophenyl propargyl ether

Inchi: InChI=1S/C9H6Cl2O/c1-2-5-12-9-4-3-7(10)6-8(9)11/h1,3-4,6H,5H2
InchiKey: KEIKGHHJUQTGSZ-UHFFFAOYSA-N
Formula: C9H6Cl2O
SMILES: C#CCOc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 201.05
CAS: 17061-90-4

Physical Properties

Property code	Value	Unit	Source
gf	212.26	kJ/mol	Joback Method
hf	112.70	kJ/mol	Joback Method
hfus	24.89	kJ/mol	Joback Method
hvap	50.27	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.005		Crippen Method
mcvol	135.660	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	529.36	K	Joback Method
tc	765.22	K	Joback Method
tf	371.69	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.36	J/mol×K	529.36	Joback Method
cpg	265.13	J/mol×K	568.67	Joback Method
cpg	274.29	J/mol×K	607.98	Joback Method
cpg	282.85	J/mol×K	647.29	Joback Method
cpg	290.85	J/mol×K	686.60	Joback Method
cpg	298.29	J/mol×K	725.91	Joback Method
cpg	305.20	J/mol×K	765.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17061904&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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