

Acetic acid, (3,5-dichlorophenyl)methyl ester

Inchi: InChI=1S/C9H8Cl2O2/c1-6(12)13-5-7-2-8(10)4-9(11)3-7/h2-4H,5H2,1H3
InchiKey: AUBLCENCKCEUKL-UHFFFAOYSA-N
Formula: C9H8Cl2O2
SMILES: CC(=O)OCc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 219.06
CAS: 85263-04-3

Physical Properties

Property code	Value	Unit	Source
gf	-139.73	kJ/mol	Joback Method
hf	-291.78	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	57.15	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.056		Crippen Method
mcvol	145.830	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1513.00		NIST Webbook
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tb	593.11	K	Joback Method
tc	820.29	K	Joback Method
tf	374.65	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.99	J/molxK	593.11	Joback Method
cpg	313.48	J/molxK	630.97	Joback Method
cpg	323.31	J/molxK	668.84	Joback Method
cpg	332.51	J/molxK	706.70	Joback Method
cpg	341.08	J/molxK	744.56	Joback Method
cpg	349.03	J/molxK	782.43	Joback Method
cpg	356.37	J/molxK	820.29	Joback Method

dvisc	0.0012799	Paxs	374.65	Joback Method
dvisc	0.0008364	Paxs	411.06	Joback Method
dvisc	0.0005857	Paxs	447.47	Joback Method
dvisc	0.0004328	Paxs	483.88	Joback Method
dvisc	0.0003336	Paxs	520.29	Joback Method
dvisc	0.0002661	Paxs	556.70	Joback Method
dvisc	0.0002182	Paxs	593.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85263043&Units=SI
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

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
mvol:	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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