

Methacrylic acid, 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C10H7Cl3O2/c1-5(2)10(14)15-9-7(12)3-6(11)4-8(9)13/h3-4H,1H2,2H3
InchiKey:	DGZZQOZXBPFEIY-UHFFFAOYSA-N
Formula:	C10H7Cl3O2
SMILES:	<chem>C=C(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl</chem>
Mol. weight [g/mol]:	265.52
CAS:	18967-27-6

Physical Properties

Property code	Value	Unit	Source
gf	-73.58	kJ/mol	Joback Method
hf	-223.99	kJ/mol	Joback Method
hfus	27.32	kJ/mol	Joback Method
hvap	63.84	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.128		Crippen Method
mcvol	167.860	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	654.96	K	Joback Method
tc	890.74	K	Joback Method
tf	412.64	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.05	J/molxK	654.96	Joback Method
cpg	357.77	J/molxK	694.26	Joback Method
cpg	366.80	J/molxK	733.55	Joback Method
cpg	375.17	J/molxK	772.85	Joback Method
cpg	382.87	J/molxK	812.15	Joback Method
cpg	389.94	J/molxK	851.45	Joback Method
cpg	396.39	J/molxK	890.74	Joback Method

Sources

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=C18967276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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