Benzenemethanol, «alpha»-(trichloromethyl)-, acetate

Other names: Rosacetol
«alpha»-(Trichloromethyl)benzyl acetate
Acetic acid, «alpha»-(trichloromethyl)benzyl ester
Benzyl alcohol, «alpha»-(trichloromethyl)-, acetate
Rose crystals
Trichlor phenyl methyl carbinyl acetate
Trichloromethylphenylcarbinyl acetate
Rose ester
Rosephenone
2,2,2-Trichloro-1-phenylethyl acetate
Benzenemethanol, «alpha»-(trichloromethyl)-, 1-acetate
2-Acetoxy-1,1,1-trichloro-2-phenylethane
Crystal rose
Rosetone
Rosone
NSC 165582
Rose acetate

Inchi: InChI=1S/C10H9Cl3O2/c1-7(14)15-9(10(11,12)13)8-5-3-2-4-6-8/h2-6,9H,1H3

InchiKey: JKRWZLOCPLZZEI-UHFFFAOYSA-N

Formula: C10H9Cl3O2

SMILES: CC(=O)OC(c1ccccc1)C(Cl)(Cl)Cl

Mol. weight [g/mol]: 267.54

CAS: 90-17-5

Physical Properties

Property code	Value	Unit	Source
gf	-123.58	kJ/mol	Joback Method
hf	-319.25	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	60.76	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.661		Crippen Method
mcvol	172.160	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1522.00		NIST Webbook
rinpol	1541.30		NIST Webbook
rinpol	1538.00		NIST Webbook

rinpol	1538.00		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2222.00		NIST Webbook
tb	639.79	K	Joback Method
tc	882.99	K	Joback Method
tf	378.22	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.66	J/mol×K	639.79	Joback Method
cpg	390.28	J/mol×K	680.32	Joback Method
cpg	400.87	J/mol×K	720.86	Joback Method
cpg	410.49	J/mol×K	761.39	Joback Method
cpg	419.21	J/mol×K	801.92	Joback Method
cpg	427.09	J/mol×K	842.46	Joback Method
cpg	434.21	J/mol×K	882.99	Joback Method
dvisc	0.0021411	Pa×s	378.22	Joback Method
dvisc	0.0010974	Pa×s	421.81	Joback Method
dvisc	0.0006375	Pa×s	465.41	Joback Method
dvisc	0.0004064	Pa×s	509.00	Joback Method
dvisc	0.0002782	Pa×s	552.60	Joback Method
dvisc	0.0002013	Pa×s	596.19	Joback Method
dvisc	0.0001522	Pa×s	639.79	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=C90175&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume