

«alpha»,«beta»-Dichlorostyrene

Other names:	Benzene, (1,2-dichloroethenyl)- Dichlorostyrene Dwuchlorostyren Styrene, «alpha»,«beta»-dichloro- 1,2-Dichloro-1-phenylethene 1,2-dichloro-1-phenylethylene
Inchi:	InChI=1S/C8H6Cl2/c9-6-8(10)7-4-2-1-3-5-7/h1-6H/b8-6+
InchiKey:	OQGSCHGFHOSXFY-SOFGYWHQSA-N
Formula:	C8H6Cl2
SMILES:	ClC=C(Cl)c1ccccc1
Mol. weight [g/mol]:	173.04
CAS:	6607-45-0

Physical Properties

Property code	Value	Unit	Source
gf	176.70	kJ/mol	Joback Method
hf	104.03	kJ/mol	Joback Method
hfus	17.80	kJ/mol	Joback Method
hvap	44.49	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.463		Crippen Method
mcvol	120.000	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	1162.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1243.00		NIST Webbook
tb	488.02	K	Joback Method
tc	727.10	K	Joback Method
tf	247.14	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.12	J/mol×K	488.02	Joback Method
cpg	220.14	J/mol×K	527.87	Joback Method
cpg	230.25	J/mol×K	567.71	Joback Method
cpg	239.50	J/mol×K	607.56	Joback Method
cpg	247.97	J/mol×K	647.41	Joback Method
cpg	255.72	J/mol×K	687.25	Joback Method
cpg	262.81	J/mol×K	727.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6607450&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
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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