

2,4-Bis(chloromethyl)-1-ethylbenzene

Inchi:	InChI=1S/C10H12Cl2/c1-2-9-4-3-8(6-11)5-10(9)7-12/h3-5H,2,6-7H2,1H3
InchiKey:	BDCGIQIEFAMISP-UHFFFAOYSA-N
Formula:	C10H12Cl2
SMILES:	CCc1ccc(CCl)cc1CCl
Mol. weight [g/mol]:	203.11

Physical Properties

Property code	Value	Unit	Source
gf	102.61	kJ/mol	Joback Method
hf	-67.62	kJ/mol	Joback Method
hfus	23.31	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.727		Crippen Method
mvol	152.480	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1550.00		NIST Webbook
tb	539.70	K	Joback Method
tc	757.64	K	Joback Method
tf	313.76	K	Joback Method
vc	0.586	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.10	J/molxK	539.70	Joback Method
cpg	324.93	J/molxK	576.02	Joback Method
cpg	337.01	J/molxK	612.35	Joback Method
cpg	348.38	J/molxK	648.67	Joback Method
cpg	359.05	J/molxK	684.99	Joback Method
cpg	369.07	J/molxK	721.31	Joback Method
cpg	378.46	J/molxK	757.64	Joback Method
dvisc	0.0017643	Paxs	313.76	Joback Method

dvisc	0.0010479	Paxs	351.42	Joback Method
dvisc	0.0006884	Paxs	389.07	Joback Method
dvisc	0.0004870	Paxs	426.73	Joback Method
dvisc	0.0003645	Paxs	464.39	Joback Method
dvisc	0.0002849	Paxs	502.04	Joback Method
dvisc	0.0002304	Paxs	539.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520575&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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