

9-(Chloromethyl)anthracene

Other names:	9-Chloromethyanthracene Anthracene, 9-(chloromethyl)- ICR 448 9-Chlormethyl-anthracen
Inchi:	InChI=1S/C15H11Cl/c16-10-15-13-7-3-1-5-11(13)9-12-6-2-4-8-14(12)15/h1-9H,10H2
InchiKey:	PCVRSXXPGXRVEZ-UHFFFAOYSA-N
Formula:	C15H11Cl
SMILES:	ClCc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]:	226.70
CAS:	24463-19-2

Physical Properties

Property code	Value	Unit	Source
gf	369.94	kJ/mol	Joback Method
hf	227.06	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	60.25	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	4.732		Crippen Method
mcvol	171.770	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	654.63	K	Joback Method
tc	906.61	K	Joback Method
tf	405.59	K	Joback Method
vc	0.660	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.16	J/mol×K	654.63	Joback Method
cpg	465.80	J/mol×K	864.61	Joback Method
cpg	455.62	J/mol×K	822.62	Joback Method
cpg	444.70	J/mol×K	780.62	Joback Method
cpg	432.91	J/mol×K	738.62	Joback Method

cpg	420.11	J/mol×K	696.63	Joback Method
cpg	475.39	J/mol×K	906.61	Joback Method
dvisc	0.0004664	Paxs	654.63	Joback Method
dvisc	0.0005296	Paxs	613.12	Joback Method
dvisc	0.0006127	Paxs	571.62	Joback Method
dvisc	0.0007251	Paxs	530.11	Joback Method
dvisc	0.0008831	Paxs	488.60	Joback Method
dvisc	0.0011156	Paxs	447.10	Joback Method
dvisc	0.0014783	Paxs	405.59	Joback Method

Sources

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=C24463192&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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