

Anisole, p(«alpha»-chloro-p-methylbenzyl)-

Inchi:	InChI=1S/C15H15ClO/c1-11-3-5-12(6-4-11)15(16)13-7-9-14(17-2)10-8-13/h3-10,15H,1-2
InchiKey:	DTTHPHQAGIFHQE-UHFFFAOYSA-N
Formula:	C15H15ClO
SMILES:	COc1ccc(C(Cl)c2ccc(C)cc2)cc1
Mol. weight [g/mol]:	246.73
CAS:	7525-21-5

Physical Properties

Property code	Value	Unit	Source
gf	161.61	kJ/mol	Joback Method
hf	-56.05	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	61.27	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.332		Crippen Method
mcvol	192.800	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
tb	665.33	K	Joback Method
tc	906.47	K	Joback Method
tf	373.84	K	Joback Method
vc	0.721	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.37	J/mol×K	665.33	Joback Method
cpg	491.68	J/mol×K	705.52	Joback Method
cpg	506.79	J/mol×K	745.71	Joback Method
cpg	520.73	J/mol×K	785.90	Joback Method
cpg	533.55	J/mol×K	826.09	Joback Method
cpg	545.31	J/mol×K	866.28	Joback Method
cpg	556.06	J/mol×K	906.47	Joback Method
dvisc	0.0012143	Paxs	373.84	Joback Method
dvisc	0.0006526	Paxs	422.42	Joback Method

dvisc	0.0003987	Paxs	471.00	Joback Method
dvisc	0.0002671	Paxs	519.59	Joback Method
dvisc	0.0001916	Paxs	568.17	Joback Method
dvisc	0.0001448	Paxs	616.75	Joback Method
dvisc	0.0001140	Paxs	665.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7525215&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
mccvol:	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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