

chiloscyphene-6

Inchi:	InChI=1S/C15H26/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h8,10-12,14-15H,5-7,9H
InchiKey:	NIFDUICZRZQAPE-UHFFFAOYSA-N
Formula:	C15H26
SMILES:	CC1CCC2C(C)CC=C(C(C)C)C2C1
Mol. weight [g/mol]:	206.37

Physical Properties

Property code	Value	Unit	Source
gf	150.99	kJ/mol	Joback Method
hf	-231.62	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	49.45	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.661		Crippen Method
mcvol	196.190	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	1479.50		NIST Webbook
rinpol	1479.50		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1613.00		NIST Webbook
tb	567.52	K	Joback Method
tc	779.81	K	Joback Method
tf	270.41	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.65	J/molxK	567.52	Joback Method
cpg	547.31	J/molxK	602.90	Joback Method
cpg	570.58	J/molxK	638.28	Joback Method
cpg	592.50	J/molxK	673.67	Joback Method
cpg	613.13	J/molxK	709.05	Joback Method
cpg	632.50	J/molxK	744.43	Joback Method

cpg	650.67	J/molxK	779.81	Joback Method
dvisc	0.0023277	Paxs	270.41	Joback Method
dvisc	0.0013591	Paxs	319.93	Joback Method
dvisc	0.0009166	Paxs	369.45	Joback Method
dvisc	0.0006786	Paxs	418.96	Joback Method
dvisc	0.0005353	Paxs	468.48	Joback Method
dvisc	0.0004419	Paxs	518.00	Joback Method
dvisc	0.0003771	Paxs	567.52	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=R142120&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
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

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