

Tetrahydrotriquinacene

Inchi: InChI=1S/C10H14/c1-2-8-5-6-9-4-3-7(1)10(8)9/h1-2,7-10H,3-6H2
InchiKey: VVQPGPGAEHQIBD-UHFFFAOYSA-N
Formula: C10H14
SMILES: C1=CC2CCC3CCC1C23
Mol. weight [g/mol]: 134.22
CAS: 57595-39-8

Physical Properties

Property code	Value	Unit	Source
gf	225.72	kJ/mol	Joback Method
hf	13.00 ± 4.20	kJ/mol	NIST Webbook
hfus	16.25	kJ/mol	Joback Method
hvap	37.75	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.609		Crippen Method
mcvol	114.880	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	447.18	K	Joback Method
tc	663.03	K	Joback Method
tf	249.28	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.68	J/mol×K	447.18	Joback Method
cpg	277.50	J/mol×K	483.15	Joback Method
cpg	295.87	J/mol×K	519.13	Joback Method
cpg	312.91	J/mol×K	555.10	Joback Method
cpg	328.70	J/mol×K	591.08	Joback Method
cpg	343.35	J/mol×K	627.05	Joback Method
cpg	356.95	J/mol×K	663.03	Joback Method
dvisc	0.0004996	Pa×s	249.28	Joback Method
dvisc	0.0006099	Pa×s	282.26	Joback Method

dvisc	0.0007141	Pa×s	315.25	Joback Method
dvisc	0.0008115	Pa×s	348.23	Joback Method
dvisc	0.0009021	Pa×s	381.21	Joback Method
dvisc	0.0009859	Pa×s	414.20	Joback Method
dvisc	0.0010635	Pa×s	447.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57595398&Units=SI

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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