Bicyclo[2.2.1]hept-2-ene, 2,7,7-trimethyl-

Other names: 2,2,7-trimethyl bicyclo(2.2.1) hept-2-ene
«xi»-Fenchene
Inchi: InChI=1S/C10H16/c1-7-6-8-4-5-9(7)10(8,2)3/h6,8-9H,4-5H2,1-3H3
InchiKey: QWEFTWKQGYFNTF-UHFFFAOYSA-N
Formula: C10H16
SMILES: CC1=CC2CCC1C2(C)C
Mol. weight [g/mol]: 136.23
CAS: 514-14-7

Physical Properties

Property code	Value	Unit	Source
gf	149.85	kJ/mol	Joback Method
hf	-69.08	kJ/mol	Joback Method
hfus	11.43	kJ/mol	Joback Method
hvap	37.35	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	912.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	912.00		NIST Webbook
tb	445.66	K	Joback Method
tc	654.83	K	Joback Method
tf	267.76	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.36	J/mol×K	445.66	Joback Method
cpg	292.47	J/mol×K	480.52	Joback Method
cpg	309.23	J/mol×K	515.38	Joback Method

cpg	324.78	J/mol×K	550.25	Joback Method
cpg	339.25	J/mol×K	585.11	Joback Method
cpg	352.77	J/mol×K	619.97	Joback Method
cpg	365.49	J/mol×K	654.83	Joback Method

Sources

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=C514147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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