trans-1,1,2,4-tetramethylcyclopentane

Other names: 1,1,2-trans-4-tetramethylcyclopentane
Inchi: InChI=1S/C9H18/c1-7-5-8(2)9(3,4)6-7/h7-8H,5-6H2,1-4H3
InchiKey: AVBGIJNNMIBMQG-YUMQZZPRSA-N
Formula: C9H18
SMILES: CC1CC(C)C(C)(C)C1
Mol. weight [g/mol]: 126.24
CAS: 62016-72-2

Physical Properties

Property code	Value	Unit	Source
hfus	8.84	kJ/mol	Joback Method
ie	9.05	eV	Cheméo Relay (1.0)
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
tb	402.01	K	Cheméo Relay (1.0)
tf	201.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.44	J/mol×K	411.50	Joback Method
cpg	275.25	J/mol×K	444.63	Joback Method
cpg	292.94	J/mol×K	477.75	Joback Method
cpg	309.58	J/mol×K	510.88	Joback Method
cpg	325.27	J/mol×K	544.01	Joback Method
cpg	340.08	J/mol×K	577.14	Joback Method
cpg	354.09	J/mol×K	610.26	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62016722&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point