2,2,4-trimethyl-3-hexene

Inchi: InChI=1S/C9H18/c1-6-8(2)7-9(3,4)5/h7H,6H2,1-5H3
InchiKey: DPFRBPJIKDMNCN-BQYQJAHWSA-N
Formula: C9H18
SMILES: CCC(C)=CC(C)(C)C
Mol. weight [g/mol]: 126.24
CAS: 102877-01-0

Physical Properties

Property code	Value	Unit	Source
af	0.2907		Cheméo Relay (1.0)
gf	99.41	kJ/mol	Joback Method
hf	-126.33	kJ/mol	Cheméo Relay (1.0)
hfus	10.54	kJ/mol	Joback Method
hvap	38.31	kJ/mol	Cheméo Relay (1.0)
ie	8.49	eV	Cheméo Relay (1.0)
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
tb	401.00 ± 3.00	K	NIST Webbook
tb	403.00 ± 5.00	K	NIST Webbook
tb	405.00 ± 5.00	K	NIST Webbook
tb	387.00 ± 3.00	K	NIST Webbook
tc	557.85	K	Cheméo Relay (1.0)
tf	162.97	K	Cheméo Relay (1.0)
vc	0.490	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.53	J/mol×K	406.13	Joback Method
cpg	275.34	J/mol×K	437.13	Joback Method
cpg	290.31	J/mol×K	468.12	Joback Method
cpg	304.47	J/mol×K	499.12	Joback Method
cpg	317.87	J/mol×K	530.11	Joback Method

cpg	330.54	J/mol×K	561.11	Joback Method
cpg	342.52	J/mol×K	592.11	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102877010&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

Legend

af: Acentric Factor
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
ie: Ionization energy
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