2-Nonene, 3-methyl-, (E)-

Inchi: InChI=1S/C10H20/c1-4-6-7-8-9-10(3)5-2/h5H,4,6-9H2,1-3H3/b10-5+
InchiKey: CMLFMHBAUHOXAV-BJMVGYQFSA-N
Formula: C10H20
SMILES: CC=C(C)CCCCCC
Mol. weight [g/mol]: 140.27
CAS: 17003-99-5

Physical Properties

Property code	Value	Unit	Source
af	0.4109		Cheméo Relay (1.0)
gf	104.99	kJ/mol	Joback Method
hf	-169.94	kJ/mol	Cheméo Relay (1.0)
hfus	20.55	kJ/mol	Joback Method
hvap	50.97	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
log10ws	-5.31		Cheméo Relay (1.0)
logp	3.923		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
tb	442.59	K	Cheméo Relay (1.0)
tc	614.31	K	Cheméo Relay (1.0)
tf	199.92	K	Cheméo Relay (1.0)
vc	0.563	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.00750e+01
Coeff. B	9.73760e-01
Coeff. C	-6.06300e-04
Coeff. D	1.57000e-07

Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17003995&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

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
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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