2,9-Dimethyl-5-decyne

Inchi: InChI=1S/C12H22/c1-11(2)9-7-5-6-8-10-12(3)4/h11-12H,7-10H2,1-4H3
InchiKey: RCFYJIGZQAOTFV-UHFFFAOYSA-N
Formula: C12H22
SMILES: CC(C)CCC#CCCC(C)C
Mol. weight [g/mol]: 166.30
CAS: 19550-56-2

Physical Properties

Property code	Value	Unit	Source
gf	248.08	kJ/mol	Joback Method
hf	-29.27	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hvap	43.68	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.862		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
tb	482.08	K	Joback Method
tc	671.05	K	Joback Method
tf	301.10	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.11	J/mol×K	482.08	Joback Method
cpg	394.32	J/mol×K	513.57	Joback Method
cpg	410.79	J/mol×K	545.07	Joback Method
cpg	426.54	J/mol×K	576.56	Joback Method
cpg	441.58	J/mol×K	608.06	Joback Method
cpg	455.94	J/mol×K	639.55	Joback Method
cpg	469.65	J/mol×K	671.05	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.00	K	2.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550562&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume