3,5-Decadiyne, 2,2-dimethyl-

Inchi: InChI=1S/C12H18/c1-5-6-7-8-9-10-11-12(2,3)4/h5-7H2,1-4H3
InchiKey: WSWDDRDGHVGAMT-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCCCC#CC#CC(C)(C)C
Mol. weight [g/mol]: 162.27
CAS: 55682-73-0

Physical Properties

Property code	Value	Unit	Source
gf	458.60	kJ/mol	Joback Method
hf	244.84	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	45.31	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.230		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
tb	488.73	K	Joback Method
tc	707.29	K	Joback Method
tf	439.62	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.32	J/mol×K	488.73	Joback Method
cpg	365.42	J/mol×K	525.16	Joback Method
cpg	381.56	J/mol×K	561.58	Joback Method
cpg	396.79	J/mol×K	598.01	Joback Method
cpg	411.15	J/mol×K	634.43	Joback Method
cpg	424.69	J/mol×K	670.86	Joback Method
cpg	437.46	J/mol×K	707.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55682730&Units=SI

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume