

12-Chloro-5-dodecyne

Other names:	12-Chloro-5-dodecyne
	12-chlorododec-5-yne
Inchi:	InChI=1S/C12H21Cl/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-4,7-12H2,1H3
InchiKey:	DJJGBABLSKSRGV-UHFFFAOYSA-N
Formula:	C12H21Cl
SMILES:	CCCCC#CCCCCCCCI
Mol. weight [g/mol]:	200.75

Physical Properties

Property code	Value	Unit	Source
af	0.5174		Cheméo Relay (1.0)
gf	241.03	kJ/mol	Joback Method
hf	-61.24	kJ/mol	Cheméo Relay (1.0)
hfus	34.15	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-5.18		Cheméo Relay (1.0)
logp	4.369		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
tb	506.60	K	Cheméo Relay (1.0)
tc	712.16	K	Cheméo Relay (1.0)
tf	247.96	K	Cheméo Relay (1.0)
vc	0.682	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.19	J/mol×K	520.39	Joback Method
cpg	424.93	J/mol×K	551.46	Joback Method
cpg	439.97	J/mol×K	582.53	Joback Method
cpg	454.34	J/mol×K	613.59	Joback Method
cpg	468.07	J/mol×K	644.66	Joback Method
cpg	481.16	J/mol×K	675.73	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42513360&Units=SI

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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