Citronellyl nitrile

Inchi: InChI=1S/C10H17N/c1-9(2)5-4-6-10(3)7-8-11/h5,10H,4,6-7H2,1-3H3
InchiKey: MTDAKBBUYMYKAR-UHFFFAOYSA-N
Formula: C10H17N
SMILES: CC(C)=CCCC(C)CC#N
Mol. weight [g/mol]: 151.25

Physical Properties

Property code	Value	Unit	Source
gf	235.73	kJ/mol	Joback Method
hf	17.30	kJ/mol	Joback Method
hfus	18.53	kJ/mol	Joback Method
hvap	47.98	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.283		Crippen Method
mcvol	148.840	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1203.70		NIST Webbook
rinpol	1203.70		NIST Webbook
rinpol	1206.80		NIST Webbook
tb	533.88	K	Joback Method
tc	730.33	K	Joback Method
tf	233.41	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.42	J/mol×K	533.88	Joback Method
cpg	354.99	J/mol×K	566.62	Joback Method
cpg	367.86	J/mol×K	599.36	Joback Method
cpg	380.07	J/mol×K	632.10	Joback Method
cpg	391.65	J/mol×K	664.84	Joback Method
cpg	402.63	J/mol×K	697.59	Joback Method
cpg	413.05	J/mol×K	730.33	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=R252638&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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