

t-Butylmalononitrile

Inchi:	InChI=1S/C7H10N2/c1-7(2,3)6(4-8)5-9/h6H,1-3H3
InchiKey:	TUJPHMQZSDKRSL-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	CC(C)(C)C(C#N)C#N
Mol. weight [g/mol]:	122.17
CAS:	4210-60-0

Physical Properties

Property code	Value	Unit	Source
chs	-4250.61 ± 0.71	kJ/mol	NIST Webbook
gf	274.82	kJ/mol	Joback Method
hf	126.70 ± 0.54	kJ/mol	NIST Webbook
hfs	66.90 ± 0.71	kJ/mol	NIST Webbook
hfus	5.96	kJ/mol	Joback Method
hsub	59.80 ± 0.70	kJ/mol	NIST Webbook
hsub	59.80	kJ/mol	NIST Webbook
hsub	59.83 ± 0.67	kJ/mol	NIST Webbook
hvap	50.45	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.696		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	560.05	K	Joback Method
tc	782.47	K	Joback Method
tf	286.05	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.27	J/mol×K	560.05	Joback Method
cpg	264.83	J/mol×K	597.12	Joback Method
cpg	273.73	J/mol×K	634.19	Joback Method
cpg	282.04	J/mol×K	671.26	Joback Method

cpg	289.77	J/mol×K	708.33	Joback Method
cpg	296.98	J/mol×K	745.40	Joback Method
cpg	303.70	J/mol×K	782.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4210600&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

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