Ethyl(1,1-dimethylpropyl)malononitrile

Inchi: InChI=1S/C10H16N2/c1-5-9(3,4)10(6-2,7-11)8-12/h5-6H2,1-4H3
InchiKey: PGJYGIZMFMZNAZ-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CCC(C)(C)C(C#N)(C#N)CC
Mol. weight [g/mol]: 164.25
CAS: 85688-95-5

Physical Properties

Property code	Value	Unit	Source
chs	-6206.80 ± 1.70	kJ/mol	NIST Webbook
gf	305.36	kJ/mol	Joback Method
hf	61.30 ± 1.90	kJ/mol	NIST Webbook
hfs	-15.00 ± 1.70	kJ/mol	NIST Webbook
hfus	9.84	kJ/mol	Joback Method
hsub	76.23 ± 0.75	kJ/mol	NIST Webbook
hsub	76.30	kJ/mol	NIST Webbook
hsub	76.20 ± 0.80	kJ/mol	NIST Webbook
hvap	56.22	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.866		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	625.90	K	Joback Method
tc	844.90	K	Joback Method
tf	337.28	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.23	J/mol×K	808.40	Joback Method
cpg	396.24	J/mol×K	625.90	Joback Method
cpg	408.64	J/mol×K	662.40	Joback Method
cpg	420.17	J/mol×K	698.90	Joback Method

cpg	430.90	J/mol×K	735.40	Joback Method
cpg	440.89	J/mol×K	771.90	Joback Method
cpg	458.97	J/mol×K	844.90	Joback Method
hfust	19.25	kJ/mol	307.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85688955&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

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
hfust:	Enthalpy of fusion at a given temperature
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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