Meso-2,3-diethyl-2,3-dimethylsuccinonitrile

Inchi: InChI=1S/C10H16N2/c1-5-9(3,7-11)10(4,6-2)8-12/h5-6H2,1-4H3
InchiKey: YPKRPUBUHLHYRJ-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CCC(C)(C#N)C(C)(C#N)CC
Mol. weight [g/mol]: 164.25
CAS: 85688-81-9

Physical Properties

Property code	Value	Unit	Source
chs	-6188.10 ± 1.30	kJ/mol	NIST Webbook
gf	305.36	kJ/mol	Joback Method
hf	64.06	kJ/mol	NIST Webbook
hfs	-33.60 ± 1.30	kJ/mol	NIST Webbook
hfus	9.84	kJ/mol	Joback Method
hsub	97.65	kJ/mol	NIST Webbook
hsub	97.70	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	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	450.23	J/mol×K	808.40	Joback Method
cpg	458.97	J/mol×K	844.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85688819&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