Tetracyclopropylsuccinonitrile

Inchi: InChI=1S/C16H20N2/c17-9-15(11-1-2-11,12-3-4-12)16(10-18,13-5-6-13)14-7-8-14/h11-1
InchiKey: YJJFFDGLUZTUKN-UHFFFAOYSA-N
Formula: C16H20N2
SMILES: N#CC(C1CC1)(C1CC1)C(C#N)(C1CC1)C1CC1
Mol. weight [g/mol]: 240.34
CAS: 19219-01-3

Physical Properties

Property code	Value	Unit	Source
gf	598.88	kJ/mol	Joback Method
hf	537.00 ± 3.00	kJ/mol	NIST Webbook
hfs	427.00 ± 3.00	kJ/mol	NIST Webbook
hfus	17.92	kJ/mol	Joback Method
hsub	110.20 ± 1.50	kJ/mol	NIST Webbook
hsub	110.00	kJ/mol	NIST Webbook
hvap	69.23	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.646		Crippen Method
mcvol	195.620	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
tb	790.14	K	Joback Method
tc	1041.47	K	Joback Method
tf	350.65 ± 1.50	K	NIST Webbook
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.83	J/mol×K	957.69	Joback Method
cpg	719.48	J/mol×K	999.58	Joback Method
cpg	643.94	J/mol×K	790.14	Joback Method
cpg	660.13	J/mol×K	832.03	Joback Method
cpg	675.46	J/mol×K	873.92	Joback Method
cpg	690.26	J/mol×K	915.81	Joback Method

cpg	734.53	J/mol×K	1041.47	Joback Method
cps	321.80	J/mol×K	298.15	NIST Webbook
hfust	22.30	kJ/mol	390.00	NIST Webbook
hfust	22.30	kJ/mol	390.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19219013&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

cpg:	Ideal gas heat capacity
cps:	Solid phase 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