Tetraisobutylsucccinonitrile

Inchi: InChI=1S/C20H36N2/c1-15(2)9-19(13-21,10-16(3)4)20(14-22,11-17(5)6)12-18(7)8/h15-1
InchiKey: KSZZCMITDIGDPJ-UHFFFAOYSA-N
Formula: C20H36N2
SMILES: CC(C)CC(C#N)(CC(C)C)C(C#N)(CC(C)C)CC(C)C
Mol. weight [g/mol]: 304.51
CAS: 85688-86-4

Physical Properties

Property code	Value	Unit	Source
chs	-12750.70 ± 3.70	kJ/mol	NIST Webbook
gf	379.80	kJ/mol	Joback Method
hf	-111.70	kJ/mol	NIST Webbook
hfs	-264.40 ± 3.70	kJ/mol	NIST Webbook
hfus	21.65	kJ/mol	Joback Method
hsub	152.70	kJ/mol	NIST Webbook
hsub	152.70	kJ/mol	NIST Webbook
hvap	76.93	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	6.191		Crippen Method
mcvol	295.420	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
tb	852.94	K	Joback Method
tc	1061.70	K	Joback Method
tf	389.98	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.74	J/mol×K	1026.91	Joback Method
cpg	943.02	J/mol×K	852.94	Joback Method
cpg	960.17	J/mol×K	887.73	Joback Method
cpg	976.33	J/mol×K	922.53	Joback Method
cpg	991.58	J/mol×K	957.32	Joback Method

cpg	1006.02	J/mol×K	992.11	Joback Method
cpg	1032.82	J/mol×K	1061.70	Joback Method
hfust	34.31	kJ/mol	360.20	NIST Webbook

Sources

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=C85688864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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