2,2-Bis-(4-cyanatophenyl)propane

Other names: 2,2-Bis-(4-cyanatophenyl)propane
Inchi: InChI=1S/C17H14N2O2/c1-17(2,13-3-7-15(8-4-13)20-11-18)14-5-9-16(10-6-14)21-12-19
InchiKey: AHZMUXQJTGRNHT-UHFFFAOYSA-N
Formula: C17H14N2O2
SMILES: CC(C)(c1ccc(OC#N)cc1)c1ccc(OC#N)cc1
Mol. weight [g/mol]: 278.31

Physical Properties

Property code	Value	Unit	Source
hfus	25.06	kJ/mol	Joback Method
log10ws	-6.24		Cheméo Relay (1.0)
logp	3.732		Crippen Method
mcvol	217.370	ml/mol	McGowan Method
ss	391.20	J/mol×K	NIST Webbook
tf	373.02	K	Cheméo Relay (1.0)
tt	355.80 ± 0.10	K	NIST Webbook
tt	355.83 ± 0.02	K	NIST Webbook
tt	355.80 ± 0.10	K	NIST Webbook
tt	355.83 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.87	J/mol×K	1066.26	Joback Method
cpg	663.42	J/mol×K	1108.46	Joback Method
cpg	669.10	J/mol×K	1150.66	Joback Method
cpg	649.38	J/mol×K	1024.06	Joback Method
cpg	620.66	J/mol×K	897.45	Joback Method
cpg	631.34	J/mol×K	939.65	Joback Method
cpg	640.89	J/mol×K	981.85	Joback Method
cps	360.00	J/mol×K	300.00	NIST Webbook
cps	355.64	J/mol×K	298.15	NIST Webbook
hfust	26.70	kJ/mol	355.80	NIST Webbook
hfust	26.69	kJ/mol	355.83	NIST Webbook

hfust	26.70	kJ/mol	355.80	NIST Webbook
hfust	26.69	kJ/mol	355.83	NIST Webbook
sfust	74.89	J/mol×K	355.83	NIST Webbook
sfust	74.89	J/mol×K	355.83	NIST Webbook
sfust	74.90	J/mol×K	355.80	NIST Webbook
sfust	74.90	J/mol×K	355.80	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1156510&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature