3,4-Dioxymethylene-p-isopropylphenylacetonitrile

Inchi: InChI=1S/C18H15NO2/c1-2-13-3-6-15(7-4-13)16(11-19)9-14-5-8-17-18(10-14)21-12-20-
InchiKey: ZWTMYUSNQWFHAV-CXUHLZMHSA-N
Formula: C19H17NO2
SMILES: CCc1ccc(C(C#N)=Cc2ccc3c(c2)OCO3)cc1
Mol. weight [g/mol]: 291.34
CAS: 53407-80-0

Physical Properties

Property code	Value	Unit	Source
chs	-9933.78	kJ/mol	NIST Webbook
gf	397.68	kJ/mol	Joback Method
hf	125.25	kJ/mol	Joback Method
hfs	27.50	kJ/mol	NIST Webbook
hfus	42.71	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.042		Crippen Method
mcvol	214.920	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
tb	850.97	K	Joback Method
tc	1105.44	K	Joback Method
tf	504.29	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.77	J/mol×K	850.97	Joback Method
cpg	629.88	J/mol×K	893.38	Joback Method
cpg	642.17	J/mol×K	935.79	Joback Method
cpg	653.78	J/mol×K	978.20	Joback Method
cpg	664.88	J/mol×K	1020.61	Joback Method
cpg	675.61	J/mol×K	1063.03	Joback Method
cpg	686.12	J/mol×K	1105.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53407800&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
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