4-Octanoate-3,5-dichlorobenzonitrile

Inchi: InChI=1S/C15H17Cl2NO2/c1-2-3-4-5-6-7-14(19)20-15-12(16)8-11(10-18)9-13(15)17/h8-9
InchiKey: YJUYRXJNOPICDZ-UHFFFAOYSA-N
Formula: C15H17Cl2NO2
SMILES: CCCCCCCC(=O)Oc1c(Cl)cc(C#N)cc1Cl
Mol. weight [g/mol]: 314.21
CAS: 1689-98-1

Physical Properties

Property code	Value	Unit	Source
gf	34.34	kJ/mol	Joback Method
hf	-262.21	kJ/mol	Joback Method
hfus	40.17	kJ/mol	Joback Method
hvap	81.65	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.131		Crippen Method
mcvol	231.750	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
tb	837.45	K	Joback Method
tc	1056.76	K	Joback Method
tf	519.78	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.71	J/mol×K	837.45	Joback Method
cpg	633.18	J/mol×K	874.00	Joback Method
cpg	643.77	J/mol×K	910.55	Joback Method
cpg	653.50	J/mol×K	947.10	Joback Method
cpg	662.38	J/mol×K	983.66	Joback Method
cpg	670.44	J/mol×K	1020.21	Joback Method
cpg	677.70	J/mol×K	1056.76	Joback Method

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=C1689981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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