Benzonitrile, 3,5-dibromo-4-octanoyloxy-

Other names: Bromoxynil octanoate
Inchi: InChI=1S/C15H17Br2NO2/c1-2-3-4-5-6-7-14(19)20-15-12(16)8-11(10-18)9-13(15)17/h8-
InchiKey: DQKWXTIYGWPGOO-UHFFFAOYSA-N
Formula: C15H17Br2NO2
SMILES: CCCCCCCC(=O)Oc1c(Br)cc(C#N)cc1Br
Mol. weight [g/mol]: 403.11
CAS: 86702-80-9

Physical Properties

Property code	Value	Unit	Source
chs	-7946.70	kJ/mol	NIST Webbook
gf	86.84	kJ/mol	Joback Method
hf	-178.07	kJ/mol	Joback Method
hfs	-599.36	kJ/mol	NIST Webbook
hfus	42.34	kJ/mol	Joback Method
hvap	85.75	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	5.349		Crippen Method
mcvol	242.270	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	2316.00		NIST Webbook
tb	894.91	K	Joback Method
tc	1126.83	K	Joback Method
tf	579.54	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.43	J/mol×K	894.91	Joback Method
cpg	651.17	J/mol×K	933.56	Joback Method
cpg	661.06	J/mol×K	972.22	Joback Method
cpg	670.17	J/mol×K	1010.87	Joback Method
cpg	678.52	J/mol×K	1049.52	Joback Method

cpg	686.16	J/mol×K	1088.17	Joback Method
cpg	693.12	J/mol×K	1126.83	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=C86702809&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume