Bromoxynil octanoate

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

Physical Properties

Property code	Value	Unit	Source
chs	-7946.70	kJ/mol	NIST Webbook
hf	-229.96	kJ/mol	Cheméo Relay (1.0)
hfs	-599.36	kJ/mol	NIST Webbook
hfus	42.34	kJ/mol	Joback Method
hvap	96.57	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.71		Cheméo Relay (1.0)
logp	5.349		Crippen Method
mcvol	242.270	ml/mol	McGowan Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook
tb	625.07	K	Cheméo Relay (1.0)
tc	883.10	K	Cheméo Relay (1.0)
tf	355.91	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86702809&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point