

Ethiofencarb

Inchi: InChI=1S/C11H15NO2S/c1-3-15-8-9-6-4-5-7-10(9)14-11(13)12-2/h4-7H,3,8H2,1-2H3,(H,12,13)
InchiKey: HEZNVIYQEUHLNI-UHFFFAOYSA-N
Formula: C11H15NO2S
SMILES: CCSCc1ccccc1OC(=O)NC
Mol. weight [g/mol]: 225.31
CAS: 29973-13-5

Physical Properties

Property code	Value	Unit	Source
hfus	31.50	kJ/mol	Joback Method
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.658		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
tf	306.55	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.70820e+01
Coeff. B	9.26230e-01
Coeff. C	-4.52560e-04
Coeff. D	4.61000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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