

tiaprofenic acid

Inchi:	InChI=1S/C14H12O3S/c1-9(14(16)17)11-7-8-12(18-11)13(15)10-5-3-2-4-6-10/h2-9H,1H3
InchiKey:	GUHPRPJDBZHYCJ-UHFFFAOYSA-N
Formula:	C14H12O3S
SMILES:	CC(C(=O)O)c1ccc(C(=O)c2ccccc2)s1
Mol. weight [g/mol]:	260.31
CAS:	33005-95-7

Physical Properties

Property code	Value	Unit	Source
hf	-376.44	kJ/mol	Cheméo Relay (1.0)
hvap	105.21	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
log10ws	-3.02		Cheméo Relay (1.0)
logp	3.167		Crippen Method
mcvol	190.260	ml/mol	McGowan Method
pc	2535.56	kPa	Cheméo Relay (1.0, beta)
tb	632.31	K	Cheméo Relay (1.0)
tc	909.88	K	Cheméo Relay (1.0)
tf	369.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	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

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