

(1-ethoxy-1-oxopropan-2-yl) 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitroben

Inchi: InChI=1S/C19H15ClF3NO7/c1-3-29-17(25)10(2)30-18(26)13-9-12(5-6-15(13)24(27)28)3

InchiKey: CONWAEURSVPLRM-UHFFFAOYSA-N

Formula: C19H15ClF3NO7

SMILES: CCOC(=O)C(C)OC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 461.78

CAS: 77501-63-4

Physical Properties

Property code	Value	Unit	Source
hfus	55.28	kJ/mol	Joback Method
log10ws	-6.17		Cheméo Relay (1.0)
logp	5.168		Crippen Method
mcvol	286.770	ml/mol	McGowan Method
tf	318.15	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	6.18210e+01
Coeff. B	1.51350e+00
Coeff. C	-8.26840e-04
Coeff. D	1.14300e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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_Dataset/1031637
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

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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