

(2-methyl-3-phenylphenyl)methyl 3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl

Inchi: InChI=1S/C23H22ClF3O2/c1-14-16(10-7-11-17(14)15-8-5-4-6-9-15)13-29-21(28)20-18(2)
InchiKey: OMFRMAHOUUJSGP-UHFFFAOYSA-N
Formula: C23H22ClF3O2
SMILES: Cc1c(COC(=O)C2C(C=C(Cl)C(F)(F)F)C2(C)C)cccc1-c1ccccc1
Mol. weight [g/mol]: 422.87
CAS: 82657-04-3

Physical Properties

Property code	Value	Unit	Source
hfus	45.89	kJ/mol	Joback Method
log10ws	-6.85		Cheméo Relay (1.0)
logp	6.662		Crippen Method
mcvol	297.240	ml/mol	McGowan Method
tf	342.15	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	-1.27359e+02
Coeff. B	2.43496e+00
Coeff. C	-2.03062e-03
Coeff. D	6.94400e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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
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

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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