

m-anisic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C19H24O3/c1-21-17-4-2-3-16(8-17)18(20)22-12-19-9-13-5-14(10-19)7-15(6-13)
InchiKey: XEOJDIHEPZRJIJ-UHFFFAOYSA-N
Formula: C19H24O3
SMILES: COc1cccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)c1
Mol. weight [g/mol]: 300.40

Physical Properties

Property code	Value	Unit	Source
hf	-550.28	kJ/mol	Cheméo Relay (1.0)
hfus	29.67	kJ/mol	Joback Method
hvap	99.77	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
logp	4.068		Crippen Method
mcvol	235.540	ml/mol	McGowan Method
rinpol	2451.90		NIST Webbook
tb	671.72	K	Cheméo Relay (1.0)
tf	429.96	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.09	J/mol×K	784.55	Joback Method
cpg	773.42	J/mol×K	823.55	Joback Method
cpg	792.97	J/mol×K	862.54	Joback Method
cpg	811.97	J/mol×K	901.54	Joback Method
cpg	830.64	J/mol×K	940.53	Joback Method
cpg	849.21	J/mol×K	979.53	Joback Method
cpg	867.90	J/mol×K	1018.53	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292253&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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