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]: 300.39

Physical Properties

Property code	Value	Unit	Source
gf	29.91	kJ/mol	Joback Method
hf	-380.31	kJ/mol	Joback Method
hfus	29.67	kJ/mol	Joback Method
hvap	70.84	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.068		Crippen Method
mcvol	235.540	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	2451.90		NIST Webbook
rinpol	2451.90		NIST Webbook
tb	784.55	K	Joback Method
tc	1018.53	K	Joback Method
tf	507.18	K	Joback Method
vc	0.893	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume