o-Anisic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C20H26O3/c1-22-18-5-3-2-4-17(18)19(21)23-7-6-20-11-14-8-15(12-20)10-16(9
InchiKey: IFNXVXHTDVOPQW-UHFFFAOYSA-N
Formula: C20H26O3
SMILES: COc1ccccc1C(=O)OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 314.42

Physical Properties

Property code	Value	Unit	Source
gf	38.33	kJ/mol	Joback Method
hf	-400.95	kJ/mol	Joback Method
hfus	32.26	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.459		Crippen Method
mcvol	249.630	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2527.00		NIST Webbook
tb	807.43	K	Joback Method
tc	1037.73	K	Joback Method
tf	518.45	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.72	J/mol×K	807.43	Joback Method
cpg	832.39	J/mol×K	845.81	Joback Method
cpg	852.36	J/mol×K	884.20	Joback Method
cpg	871.85	J/mol×K	922.58	Joback Method
cpg	891.07	J/mol×K	960.96	Joback Method
cpg	910.25	J/mol×K	999.34	Joback Method
cpg	929.61	J/mol×K	1037.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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