1-Adamantanecarboxylic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C19H24O2/c1-12-3-13(2)5-17(4-12)21-18(20)19-9-14-6-15(10-19)8-16(7-14)11

InchiKey: FQRPDLFZZYNVAZ-UHFFFAOYSA-N

Formula: C19H24O2

SMILES: Cc1cc(C)cc(OC(=O)C23CC4CC(CC(C4)C2)C3)c1

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	125.28	kJ/mol	Joback Method
hf	-259.56	kJ/mol	Joback Method
hfus	28.09	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.425		Crippen Method
mcvol	229.670	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2240.00		NIST Webbook
tb	767.11	K	Joback Method
tc	1004.92	K	Joback Method
tf	497.47	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.96	J/mol×K	767.11	Joback Method
cpg	743.66	J/mol×K	806.75	Joback Method
cpg	763.54	J/mol×K	846.38	Joback Method
cpg	782.84	J/mol×K	886.02	Joback Method
cpg	801.83	J/mol×K	925.65	Joback Method
cpg	820.75	J/mol×K	965.29	Joback Method
cpg	839.84	J/mol×K	1004.92	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=U307661&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