1-Adamantanecarboxylic acid, 3-methylphenyl ester

Inchi: InChI=1S/C18H22O2/c1-12-3-2-4-16(5-12)20-17(19)18-9-13-6-14(10-18)8-15(7-13)11-18
InchiKey: DYVRJWFCGLMSCP-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: Cc1cccc(OC(=O)C23CC4CC(CC(C4)C2)C3)c1
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
gf	126.49	kJ/mol	Joback Method
hf	-227.45	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	66.21	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.117		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	2134.00		NIST Webbook
tb	739.25	K	Joback Method
tc	980.95	K	Joback Method
tf	473.68	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.49	J/mol×K	739.25	Joback Method
cpg	686.95	J/mol×K	779.53	Joback Method
cpg	706.45	J/mol×K	819.82	Joback Method
cpg	725.25	J/mol×K	860.10	Joback Method
cpg	743.62	J/mol×K	900.38	Joback Method
cpg	761.83	J/mol×K	940.67	Joback Method
cpg	780.13	J/mol×K	980.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307659&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

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