5,7-dimethyladamantane-1,3-dicarboxylic acid, dimethyl ester

Inchi: InChI=1S/C16H24O4/c1-13-5-14(2)8-15(6-13,11(17)19-3)10-16(7-13,9-14)12(18)20-4/h5

InchiKey: VFSOMLCPYKZNBM-SYMSYNOKSA-N

Formula: C16H24O4

SMILES: COC(=O)C12CC3(C)CC(C)(C1)CC(C(=O)OC)(C3)C2

Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	-243.52	kJ/mol	Joback Method
hf	-610.31	kJ/mol	Joback Method
hfus	10.95	kJ/mol	Joback Method
hvap	64.52	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.699		Crippen Method
mcvol	218.600	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1769.00		NIST Webbook
tb	738.84	K	Joback Method
tc	972.99	K	Joback Method
tf	556.06	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.52	J/mol×K	738.84	Joback Method
cpg	695.66	J/mol×K	777.86	Joback Method
cpg	716.36	J/mol×K	816.89	Joback Method
cpg	738.16	J/mol×K	855.91	Joback Method
cpg	761.58	J/mol×K	894.94	Joback Method
cpg	787.14	J/mol×K	933.96	Joback Method

cpg	815.39	J/mol×K	972.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304902&Units=SI

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