Adamantane, 3,7-dimethyl-, 1,5-dicarboxylic acid, dipentyl ester

Inchi: InChI=1S/C24H40O4/c1-5-7-9-11-27-19(25)23-14-21(3)13-22(4,15-23)17-24(16-21,18-2

InchiKey: HBCLIUNHVUWZBQ-UHFFFAOYSA-N

Formula: C24H40O4

SMILES: CCCCCOC(=O)C12CC3(C)CC(C)(C1)CC(C(=O)OCCCCC)(C3)C2

Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-176.16	kJ/mol	Joback Method
hf	-775.43	kJ/mol	Joback Method
hfus	31.67	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.820		Crippen Method
mcvol	331.320	ml/mol	McGowan Method
pc	1215.74	kPa	Joback Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	921.88	K	Joback Method
tc	1139.57	K	Joback Method
tf	646.22	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.05	J/mol×K	921.88	Joback Method
cpg	1209.44	J/mol×K	958.16	Joback Method
cpg	1244.00	J/mol×K	994.44	Joback Method
cpg	1281.19	J/mol×K	1030.72	Joback Method
cpg	1321.46	J/mol×K	1067.00	Joback Method
cpg	1365.26	J/mol×K	1103.29	Joback Method
cpg	1413.05	J/mol×K	1139.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407485&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

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