Tricyclo[3.3.1.1(3,7)]decane-2,4-dione

Other names: 2,4-Adamantanedione
Tricyclo[3.3.1.1(3,7)]decane-2,4-dione
Adamantan-2,4-dione
Inchi: InChI=1S/C10H12O2/c11-9-6-1-5-2-7(4-6)10(12)8(9)3-5/h5-8H,1-4H2
InchiKey: FSLRANFXEMHCCW-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: O=C1C2CC3CC(C2)C(=O)C1C3
Mol. weight [g/mol]: 164.20

Physical Properties

Property code	Value	Unit	Source
hf	-337.47	kJ/mol	Cheméo Relay (1.0)
hfus	14.05	kJ/mol	Joback Method
hvap	64.49	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
logp	1.191		Crippen Method
mcvol	122.320	ml/mol	McGowan Method
rinpol	1539.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1551.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.99	J/mol×K	583.66	Joback Method
cpg	361.57	J/mol×K	624.70	Joback Method
cpg	378.93	J/mol×K	665.73	Joback Method
cpg	395.12	J/mol×K	706.77	Joback Method
cpg	410.19	J/mol×K	747.81	Joback Method
cpg	424.18	J/mol×K	788.85	Joback Method
cpg	437.16	J/mol×K	829.88	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19214007&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices