3-Cyclopentylpropionic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C20H32O2/c21-19(6-5-15-3-1-2-4-15)22-8-7-20-12-16-9-17(13-20)11-18(10-16

InchiKey: YYNSVXZFHKVVBJ-UHFFFAOYSA-N

Formula: C20H32O2

SMILES: O=C(CCC1CCCC1)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	77.10	kJ/mol	Joback Method
hf	-433.31	kJ/mol	Joback Method
hfus	31.36	kJ/mol	Joback Method
hvap	67.98	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.107		Crippen Method
mcvol	256.660	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	2391.00		NIST Webbook
tb	768.63	K	Joback Method
tc	989.02	K	Joback Method
tf	468.18	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.21	J/mol×K	768.63	Joback Method
cpg	883.69	J/mol×K	805.36	Joback Method
cpg	906.18	J/mol×K	842.09	Joback Method
cpg	927.91	J/mol×K	878.82	Joback Method
cpg	949.10	J/mol×K	915.55	Joback Method
cpg	969.96	J/mol×K	952.29	Joback Method
cpg	990.72	J/mol×K	989.02	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=U292270&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