3-Cyclopentylpropionic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C19H30O2/c20-18(6-5-14-3-1-2-4-14)21-13-19-10-15-7-16(11-19)9-17(8-15)12

InchiKey: HTFKCXOAQAOCKI-UHFFFAOYSA-N

Formula: C19H30O2

SMILES: O=C(CCC1CCCC1)OCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	68.68	kJ/mol	Joback Method
hf	-412.67	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.716		Crippen Method
mcvol	242.570	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	2263.40		NIST Webbook
tb	745.75	K	Joback Method
tc	969.41	K	Joback Method
tf	456.91	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.37	J/mol×K	745.75	Joback Method
cpg	823.70	J/mol×K	783.03	Joback Method
cpg	845.96	J/mol×K	820.30	Joback Method
cpg	867.37	J/mol×K	857.58	Joback Method
cpg	888.15	J/mol×K	894.86	Joback Method
cpg	908.53	J/mol×K	932.13	Joback Method
cpg	928.74	J/mol×K	969.41	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=U292269&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