4-(2,7,7-Trimethylbicyclo[3.2.1]hept-2-en-1-yl]but-

Inchi: InChI=1S/C15H22O/c1-11-5-6-13-8-10-15(11,14(13,3)4)9-7-12(2)16/h5,7,9,13H,6,8,10H
InchiKey: AYJXQXRELKDGNE-VQHVLOKHSA-N
Formula: C15H22O
SMILES: CC(=O)C=CC12CCC(CC=C1C)C2(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	125.66	kJ/mol	Joback Method
hf	-158.56	kJ/mol	Joback Method
hfus	17.79	kJ/mol	Joback Method
hvap	54.20	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1472.00		NIST Webbook
tb	622.60	K	Joback Method
tc	849.19	K	Joback Method
tf	389.34	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.99	J/mol×K	622.60	Joback Method
cpg	542.14	J/mol×K	660.36	Joback Method
cpg	560.25	J/mol×K	698.13	Joback Method
cpg	577.58	J/mol×K	735.89	Joback Method
cpg	594.45	J/mol×K	773.66	Joback Method
cpg	611.12	J/mol×K	811.42	Joback Method
cpg	627.90	J/mol×K	849.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R635102&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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