

exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl isobutyrate

Other names:	(1R,2R,4R)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl isobutyrate
Inchi:	InChI=1S/C14H24O2/c1-9(2)12(15)16-11-8-10-6-7-14(11,5)13(10,3)4/h9-11H,6-8H2,1-5H
InchiKey:	KRKIAJBQOUBNSE-COPLHBTASA-N
Formula:	C14H24O2
SMILES:	CC(C)C(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	224.34
CAS:	85586-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-86.36	kJ/mol	Joback Method
hf	-453.13	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	52.60	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.400		Crippen Method
mcvol	193.840	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1418.20		NIST Webbook
rinpol	1418.20		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1641.00		NIST Webbook
tb	604.46	K	Joback Method
tc	817.37	K	Joback Method
tf	376.38	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.35	J/mol×K	604.46	Joback Method
cpg	560.28	J/mol×K	639.94	Joback Method
cpg	579.13	J/mol×K	675.43	Joback Method
cpg	597.14	J/mol×K	710.91	Joback Method

cpg	614.49	J/mol×K	746.40	Joback Method
cpg	631.42	J/mol×K	781.88	Joback Method
cpg	648.14	J/mol×K	817.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85586670&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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