

(E)-6-(2,3-dimethyltricyclo[2.2.1.0^{2,6}]heptan-3-yl)-

Inchi: InChI=1S/C16H24O/c1-10(11(2)17)6-5-7-15(3)12-8-13-14(9-12)16(13,15)4/h6,12-14H,5,
InchiKey: AJAXBERBECDKTL-UXBLZVDNSA-N
Formula: C16H24O
SMILES: CC(=O)C(C)=CCCC1(C)C2CC3C(C2)C31C
Mol. weight [g/mol]: 232.36

Physical Properties

Property code	Value	Unit	Source
gf	206.64	kJ/mol	Joback Method
hf	-158.20	kJ/mol	Joback Method
hfus	25.84	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.984		Crippen Method
mcvol	200.990	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1866.60		NIST Webbook
rinpol	1866.60		NIST Webbook
tb	626.21	K	Joback Method
tc	836.24	K	Joback Method
tf	401.15	K	Joback Method
vc	0.799	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.44	J/mol×K	626.21	Joback Method
cpg	595.05	J/mol×K	661.21	Joback Method
cpg	612.66	J/mol×K	696.22	Joback Method
cpg	629.56	J/mol×K	731.22	Joback Method
cpg	646.04	J/mol×K	766.23	Joback Method
cpg	662.38	J/mol×K	801.23	Joback Method
cpg	678.88	J/mol×K	836.24	Joback Method

Sources

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=U412718&Units=SI
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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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