Prohydrojasmon, isomer 2

Inchi: InChI=1S/C15H26O3/c1-3-5-6-7-13-12(8-9-14(13)16)11-15(17)18-10-4-2/h12-13H,3-11H
InchiKey: IPDFPNNPBMREIF-UHFFFAOYSA-N
Formula: C15H26O3
SMILES: CCCCCC1C(=O)CCC1CC(=O)OCCC
Mol. weight [g/mol]: 254.37

Physical Properties

Property code	Value	Unit	Source
gf	-252.25	kJ/mol	Joback Method
hf	-695.29	kJ/mol	Joback Method
hfus	31.91	kJ/mol	Joback Method
hvap	62.33	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.505		Crippen Method
mcvol	220.360	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	1844.00		NIST Webbook
rinpol	1844.00		NIST Webbook
tb	697.32	K	Joback Method
tc	895.13	K	Joback Method
tf	405.85	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.85	J/mol×K	697.32	Joback Method
cpg	673.87	J/mol×K	730.29	Joback Method
cpg	691.83	J/mol×K	763.26	Joback Method
cpg	708.74	J/mol×K	796.23	Joback Method
cpg	724.59	J/mol×K	829.19	Joback Method
cpg	739.38	J/mol×K	862.16	Joback Method
cpg	753.12	J/mol×K	895.13	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=R566660&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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