Pentadeca-1,3,7,12,14-pentaen-7-ol-9-one

Inchi: InChI=1S/C15H20O2/c1-3-5-7-9-11-14(16)13-15(17)12-10-8-6-4-2/h3-8,13,16H,1-2,9-12
InchiKey: VKIXTEBVBVMACG-LBPZLPHVSA-N
Formula: C15H20O2
SMILES: C=CC=CCCC(=O)C=C(O)CCC=CC=C
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	217.47	kJ/mol	Joback Method
hf	-25.01	kJ/mol	Joback Method
hfus	37.03	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.042		Crippen Method
mcvol	208.150	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	694.37	K	Joback Method
tc	881.36	K	Joback Method
tf	336.84	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.91	J/mol×K	694.37	Joback Method
cpg	560.76	J/mol×K	725.54	Joback Method
cpg	572.94	J/mol×K	756.70	Joback Method
cpg	584.51	J/mol×K	787.87	Joback Method
cpg	595.52	J/mol×K	819.03	Joback Method
cpg	606.05	J/mol×K	850.20	Joback Method
cpg	616.16	J/mol×K	881.36	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=U161456&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