Oxacycloheptadec-8-en-2-one, (8Z)-

Other names:	Musk ambrette
	Ambrettolid
	Ambrettolide
	Musk ambrette, natural
	Musk natural
	Oxacycloheptadec-8-en-2-one, (Z)-
	Natural musk ambrette
	(Z)-7-Hexadecen-16-olide
	16-Hydroxy-7-hexadecenoic acid lactone, cis-
	hexadec-7-en-16-olide
Inchi:	InChI=1S/C16H28O2/c17-16-14-12-10-8-6-4-2-1-3-5-7-9-11-13-15-18-16/h2,4H,1,3,5-15
InchiKey:	NVIPUOMWGQAOIT-RQOWECAXSA-N
Formula:	C16H28O2
SMILES:	O=C1CCCCCC=CCCCCCCCCO1
Mol. weight [g/mol]:	252.39
CAS:	123-69-3

Physical Properties

Property code	Value	Unit	Source
gf	-195.85	kJ/mol	Joback Method
hf	-578.59	kJ/mol	Joback Method
hfus	13.57	kJ/mol	Joback Method
hvap	62.89	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.781		Crippen Method
mcvol	228.580	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	1927.50		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1927.50		NIST Webbook
ripol	2475.00		NIST Webbook
ripol	2475.00		NIST Webbook
tb	730.60	K	Joback Method
tc	1003.49	K	Joback Method
tf	338.53	K	Joback Method

vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.37	J/mol×K	730.60	Joback Method
cpg	732.68	J/mol×K	776.08	Joback Method
cpg	758.95	J/mol×K	821.56	Joback Method
cpg	782.04	J/mol×K	867.04	Joback Method
cpg	801.83	J/mol×K	912.52	Joback Method
cpg	818.18	J/mol×K	958.01	Joback Method
cpg	830.97	J/mol×K	1003.49	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C123693&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume