2H-Pyran, 2-(7-heptadecynyloxy)tetrahydro-

Inchi: InChI=1S/C22H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23-22-19-16-18-21-24
InchiKey: ONANHJGDQJCYMD-UHFFFAOYSA-N
Formula: C22H40O2
SMILES: CCCCCCCCCC#CCCCCCCOC1CCCCO1
Mol. weight [g/mol]: 336.55
CAS: 56599-50-9

Physical Properties

Property code	Value	Unit	Source
gf	170.49	kJ/mol	Joback Method
hf	-435.01	kJ/mol	Joback Method
hfus	56.86	kJ/mol	Joback Method
hvap	74.07	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.624		Crippen Method
mcvol	313.120	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
tb	780.68	K	Joback Method
tc	973.22	K	Joback Method
tf	499.98	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.56	J/mol×K	780.68	Joback Method
cpg	1012.45	J/mol×K	812.77	Joback Method
cpg	1033.09	J/mol×K	844.86	Joback Method
cpg	1052.51	J/mol×K	876.95	Joback Method
cpg	1070.74	J/mol×K	909.04	Joback Method
cpg	1087.83	J/mol×K	941.13	Joback Method
cpg	1103.80	J/mol×K	973.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56599509&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume