Sucrose Octaacetate

Other names:	«alpha»-D-Glucopyranoside, 1,3,4,6-tetra-O-acetyl-«beta»-D-fructofuranosyl, tetraacetate Octaacetyl sucrose D-(+)-Sucrose octaacetate Saccharose octaacetate Soa
Inchi:	InChI=1S/C28H38O19/c1-12(29)37-9-20-22(40-15(4)32)24(42-17(6)34)25(43-18(7)35)27
InchiKey:	ZIJKGAXBCRWEOL-UHFFFAOYSA-N
Formula:	C28H38O19
SMILES:	CC(=O)OCC1OC(OC2(COC(C)=O)OC(COC(C)=O)C(OC(C)=O)C2OC(C)=O)C(OC(C)=C
Mol. weight [g/mol]:	678.59
CAS:	126-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-1962.18	kJ/mol	Joback Method
hf	-2988.21	kJ/mol	Joback Method
hfus	94.69	kJ/mol	Joback Method
hvap	159.97	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	-0.829		Crippen Method
mcvol	460.790	ml/mol	McGowan Method
pc	878.44	kPa	Joback Method
tb	1529.06	K	Joback Method
tc	2046.05	K	Joback Method
tf	360.00 ± 4.00	K	NIST Webbook
vc	1.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1590.07	J/mol×K	1529.06	Joback Method
cpg	1527.54	J/mol×K	1615.23	Joback Method
cpg	1446.97	J/mol×K	1701.39	Joback Method
cpg	1347.92	J/mol×K	1787.56	Joback Method

cpg	1229.98	J/mol×K	1873.72	Joback Method
cpg	1092.71	J/mol×K	1959.89	Joback Method
cpg	935.70	J/mol×K	2046.05	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=C126147&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume