Benzene-hexa-n-octanoate

Inchi: InChI=1S/C54H90O12/c1-7-13-19-25-31-37-43(55)61-49-50(62-44(56)38-32-26-20-14-8-
InchiKey: ZYULWONIYVWSQP-UHFFFAOYSA-N
Formula: C54H90O12
SMILES: CCCCCCCC(=O)Oc1c(OC(=O)CCCCCCC)c(OC(=O)CCCCCCC)c(OC(=O)CCCCCCC)c
Mol. weight [g/mol]: 931.29
CAS: 65201-71-0

Physical Properties

Property code	Value	Unit	Source
gf	-935.46	kJ/mol	Joback Method
hf	-2447.51	kJ/mol	Joback Method
hfus	144.43	kJ/mol	Joback Method
hvap	196.32	kJ/mol	Joback Method
log10ws	-18.42		Crippen Method
logp	15.282		Crippen Method
mcvol	792.600	ml/mol	McGowan Method
pc	290.22	kPa	Joback Method
ss	1514.20	J/mol×K	NIST Webbook
tb	1944.24	K	Joback Method
tc	5876.36	K	Joback Method
tf	1220.32	K	Joback Method
vc	3.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2548.54	J/mol×K	1944.24	Joback Method
cpg	1379.84	J/mol×K	2599.59	Joback Method
cpg	-361.60	J/mol×K	3254.95	Joback Method
cpg	-2423.55	J/mol×K	3910.30	Joback Method
cpg	-4553.77	J/mol×K	4565.65	Joback Method
cpg	-6500.01	J/mol×K	5221.01	Joback Method
cpg	-8010.04	J/mol×K	5876.36	Joback Method
cps	2131.30	J/mol×K	298.15	NIST Webbook

dvisc	0.0000004	Pa×s	1220.32	Joback Method
dvisc	0.0000002	Pa×s	1340.97	Joback Method
dvisc	0.0000001	Pa×s	1461.63	Joback Method
dvisc	9.9603084e-08	Pa×s	1582.28	Joback Method
dvisc	7.1568293e-08	Pa×s	1702.93	Joback Method
dvisc	5.3723477e-08	Pa×s	1823.59	Joback Method
dvisc	4.1789457e-08	Pa×s	1944.24	Joback Method

Sources

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=C65201710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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