Benzene-hexa-n-heptanoate

Inchi: InChI=1S/C48H78O12/c1-7-13-19-25-31-37(49)55-43-44(56-38(50)32-26-20-14-8-2)46(5
InchiKey: XSMGMVIWGWBNBA-UHFFFAOYSA-N
Formula: C48H78O12
SMILES: CCCCCCC(=O)Oc1c(OC(=O)CCCCCC)c(OC(=O)CCCCCC)c(OC(=O)CCCCCC)c(OC(=
Mol. weight [g/mol]: 847.13
CAS: 65201-70-9

Physical Properties

Property code	Value	Unit	Source
gf	-985.98	kJ/mol	Joback Method
hf	-2323.67	kJ/mol	Joback Method
hfus	128.89	kJ/mol	Joback Method
hvap	182.96	kJ/mol	Joback Method
log10ws	-15.91		Crippen Method
logp	12.941		Crippen Method
mcvol	708.060	ml/mol	McGowan Method
pc	356.81	kPa	Joback Method
ss	1530.10	J/mol×K	NIST Webbook
tb	1806.96	K	Joback Method
tc	3795.33	K	Joback Method
tf	1152.70	K	Joback Method
vc	2.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2317.23	J/mol×K	1806.96	Joback Method
cpg	1857.95	J/mol×K	2138.36	Joback Method
cpg	1177.90	J/mol×K	2469.75	Joback Method
cpg	294.12	J/mol×K	2801.15	Joback Method
cpg	-776.38	J/mol×K	3132.54	Joback Method
cpg	-2016.57	J/mol×K	3463.94	Joback Method
cpg	-3409.43	J/mol×K	3795.33	Joback Method
cps	1505.00	J/mol×K	298.15	NIST Webbook

cps	1500.00	J/mol×K	300.00	NIST Webbook
dvisc	0.0000010	Pa×s	1152.70	Joback Method
dvisc	0.0000006	Pa×s	1261.74	Joback Method
dvisc	0.0000004	Pa×s	1370.79	Joback Method
dvisc	0.0000003	Pa×s	1479.83	Joback Method
dvisc	0.0000002	Pa×s	1588.87	Joback Method
dvisc	0.0000002	Pa×s	1697.92	Joback Method
dvisc	0.0000001	Pa×s	1806.96	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65201709&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

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