1,2,4-Benzenetricarboxylic acid, tridecyl ester (iso)

Other names: tridecyl benzene-1,2,4-tricarboxylate
Inchi: InChI=1S/C39H66O6/c1-4-7-10-13-16-19-22-25-30-43-37(40)34-28-29-35(38(41)44-31-2
InchiKey: SMYKBXMWXCZOLU-UHFFFAOYSA-N
Formula: C39H66O6
SMILES: CCCCCCCCCCOC(=O)c1ccc(C(=O)OCCCCCCCCCC)c(C(=O)OCCCCCCCCCC)c1
Mol. weight [g/mol]: 630.94
CAS: 4130-35-2

Physical Properties

Property code	Value	Unit	Source
gf	-331.11	kJ/mol	Joback Method
hf	-1369.10	kJ/mol	Joback Method
hfus	98.39	kJ/mol	Joback Method
hvap	133.48	kJ/mol	Joback Method
log10ws	-13.50		Crippen Method
logp	11.579		Crippen Method
mcvol	558.930	ml/mol	McGowan Method
pc	488.82	kPa	Joback Method
tb	1357.23	K	Joback Method
tc	1870.49	K	Joback Method
tf	797.23	K	Joback Method
vc	2.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2089.24	J/mol×K	1357.23	Joback Method
cpg	2100.83	J/mol×K	1442.77	Joback Method
cpg	2103.94	J/mol×K	1528.32	Joback Method
cpg	2099.46	J/mol×K	1613.86	Joback Method
cpg	2088.27	J/mol×K	1699.40	Joback Method
cpg	2071.28	J/mol×K	1784.94	Joback Method
cpg	2049.36	J/mol×K	1870.49	Joback Method
dvisc	0.0000257	Pa×s	797.23	Joback Method

dvisc	0.0000133	Pa×s	890.56	Joback Method
dvisc	0.0000078	Pa×s	983.90	Joback Method
dvisc	0.0000050	Pa×s	1077.23	Joback Method
dvisc	0.0000035	Pa×s	1170.56	Joback Method
dvisc	0.0000025	Pa×s	1263.90	Joback Method
dvisc	0.0000019	Pa×s	1357.23	Joback Method

Sources

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=C4130352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume