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

Inchi: InChI=1S/C33H54O6/c1-4-7-10-13-16-19-24-37-31(34)28-22-23-29(32(35)38-25-20-17-1

InchiKey: JNXDCMUUZNIWPQ-UHFFFAOYSA-N

Formula: C33H54O6

SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)OCCCCCCCC)c(C(=O)OCCCCCCCC)c1

Mol. weight [g/mol]: 546.78

Physical Properties

Property code	Value	Unit	Source
gf	-381.63	kJ/mol	Joback Method
hf	-1245.26	kJ/mol	Joback Method
hfus	82.85	kJ/mol	Joback Method
hvap	120.12	kJ/mol	Joback Method
log10ws	-10.99		Crippen Method
logp	9.239		Crippen Method
mcvol	474.390	ml/mol	McGowan Method
pc	641.90	kPa	Joback Method
tb	1219.95	K	Joback Method
tc	1561.56	K	Joback Method
tf	729.61	K	Joback Method
vc	1.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1716.89	J/mol×K	1219.95	Joback Method
cpg	1730.99	J/mol×K	1276.89	Joback Method
cpg	1740.91	J/mol×K	1333.82	Joback Method
cpg	1746.83	J/mol×K	1390.76	Joback Method
cpg	1748.94	J/mol×K	1447.69	Joback Method
cpg	1747.42	J/mol×K	1504.63	Joback Method
cpg	1742.46	J/mol×K	1561.56	Joback Method
dvisc	0.0000608	Pa×s	729.61	Joback Method
dvisc	0.0000329	Pa×s	811.33	Joback Method
dvisc	0.0000199	Pa×s	893.06	Joback Method

dvisc	0.0000131	Pa×s	974.78	Joback Method
dvisc	0.0000092	Pa×s	1056.50	Joback Method
dvisc	0.0000068	Pa×s	1138.23	Joback Method
dvisc	0.0000052	Pa×s	1219.95	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=B6010096&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
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