

1,2,4-Benzenetricarboxylic acid, trioctyl ester

Other names:	trioctyl benzene-1,2,4-tricarboxylate
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
CAS:	89-04-3

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1716.89	J/molxK	1219.95	Joback Method
cpg	1730.99	J/molxK	1276.89	Joback Method
cpg	1740.91	J/molxK	1333.82	Joback Method
cpg	1746.83	J/molxK	1390.76	Joback Method
cpg	1748.94	J/molxK	1447.69	Joback Method
cpg	1747.42	J/molxK	1504.63	Joback Method
cpg	1742.46	J/molxK	1561.56	Joback Method
dvisc	0.0000608	Paxs	729.61	Joback Method

dvisc	0.0000329	Paxs	811.33	Joback Method
dvisc	0.0000199	Paxs	893.06	Joback Method
dvisc	0.0000131	Paxs	974.78	Joback Method
dvisc	0.0000092	Paxs	1056.50	Joback Method
dvisc	0.0000068	Paxs	1138.23	Joback Method
dvisc	0.0000052	Paxs	1219.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C89043&Units=SI

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

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