Tetracosyl benzoate

Inchi: InChI=1S/C31H54O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-26-29
InchiKey: XEJNCYYPJMMJGL-UHFFFAOYSA-N
Formula: C31H54O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 458.76
CAS: 103569-99-9

Physical Properties

Property code	Value	Unit	Source
gf	88.63	kJ/mol	Joback Method
hf	-691.44	kJ/mol	Joback Method
hfus	72.87	kJ/mol	Joback Method
hvap	96.03	kJ/mol	Joback Method
log10ws	-11.34		Crippen Method
logp	10.445		Crippen Method
mcvol	431.330	ml/mol	McGowan Method
pc	686.37	kPa	Joback Method
rinpol	3459.50		NIST Webbook
rinpol	3459.50		NIST Webbook
tb	1011.65	K	Joback Method
tc	1247.46	K	Joback Method
tf	537.71	K	Joback Method
vc	1.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1514.65	J/mol×K	1011.65	Joback Method
cpg	1610.95	J/mol×K	1208.16	Joback Method
cpg	1594.67	J/mol×K	1168.86	Joback Method
cpg	1577.01	J/mol×K	1129.55	Joback Method
cpg	1557.87	J/mol×K	1090.25	Joback Method
cpg	1537.12	J/mol×K	1050.95	Joback Method
cpg	1625.98	J/mol×K	1247.46	Joback Method

dvisc	0.0000149	Pa×s	1011.65	Joback Method
dvisc	0.0000202	Pa×s	932.66	Joback Method
dvisc	0.0000290	Pa×s	853.67	Joback Method
dvisc	0.0000447	Pa×s	774.68	Joback Method
dvisc	0.0000761	Pa×s	695.69	Joback Method
dvisc	0.0001484	Pa×s	616.70	Joback Method
dvisc	0.0003525	Pa×s	537.71	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=C103569999&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume