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
af	1.3259		Cheméo Relay (1.0)
hf	-755.08	kJ/mol	Cheméo Relay (1.0)
hfus	74.46	kJ/mol	Joback Method
hvap	149.87	kJ/mol	Cheméo Relay (1.0)
ie	9.73	eV	Cheméo Relay (1.0)
log10ws	-9.86		Cheméo Relay (1.0)
logp	10.445		Crippen Method
mcvol	431.330	ml/mol	McGowan Method
pc	671.85	kPa	Joback Method
rinpol	3459.50		NIST Webbook
rinpol	3459.50		NIST Webbook
tb	690.46	K	Cheméo Relay (1.0)
tc	894.22	K	Cheméo Relay (1.0)
tf	315.10	K	Cheméo Relay (1.0)
vc	1.664	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-3.37870e+01
Coeff. B	2.81512e+00
Coeff. C	-1.59920e-03

Coeff. D	3.26100e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.49334e+01
Coeff. B	3.65254e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	507.88
Temperature range (K), max.	856.76

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103569999&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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