Benzyl docosanoate

Inchi: InChI=1S/C29H50O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-26-29(30)31
InchiKey: FYOGVGKALAEVBF-UHFFFAOYSA-N
Formula: C29H50O2
SMILES: CCCCCCCCCCCCCCCCCCCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 430.72

Physical Properties

Property code	Value	Unit	Source
af	1.2238		Cheméo Relay (1.0)
gf	71.79	kJ/mol	Joback Method
hf	-703.03	kJ/mol	Cheméo Relay (1.0)
hfus	67.69	kJ/mol	Joback Method
hvap	134.25	kJ/mol	Cheméo Relay (1.0)
ie	9.35	eV	Cheméo Relay (1.0)
log10ws	-8.93		Cheméo Relay (1.0)
logp	9.552		Crippen Method
mcvol	403.150	ml/mol	McGowan Method
pc	761.00	kPa	Joback Method
rinpol	3305.80		NIST Webbook
rinpol	3305.80		NIST Webbook
tb	672.39	K	Cheméo Relay (1.0)
tc	879.71	K	Cheméo Relay (1.0)
tf	313.53	K	Cheméo Relay (1.0)
vc	1.547	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.52	J/mol×K	965.89	Joback Method
cpg	1405.79	J/mol×K	1002.36	Joback Method
cpg	1425.55	J/mol×K	1038.82	Joback Method
cpg	1443.89	J/mol×K	1075.29	Joback Method
cpg	1460.89	J/mol×K	1111.75	Joback Method
cpg	1476.64	J/mol×K	1148.22	Joback Method

cpg	1491.24	J/mol×K	1184.68	Joback Method
dvisc	0.0004593	Pa×s	515.17	Joback Method
dvisc	0.0001962	Pa×s	590.29	Joback Method
dvisc	0.0001016	Pa×s	665.41	Joback Method
dvisc	0.0000601	Pa×s	740.53	Joback Method
dvisc	0.0000392	Pa×s	815.65	Joback Method
dvisc	0.0000274	Pa×s	890.77	Joback Method
dvisc	0.0000203	Pa×s	965.89	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85263747&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
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