Docosanoic acid, docosyl ester

Other names:	Behenyl behenate
	Starfol BB
	Docosyl docosanoate
	Docosanyl docosanoate
	Docosyl behenate
	Pelemol BB
	Kester Wax 72
Inchi:	InChI=1S/C44H88O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-
InchiKey:	NJIMZDGGLTUCPX-UHFFFAOYSA-N
Formula:	C44H88O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	649.17
CAS:	17671-27-1

Physical Properties

Property code	Value	Unit	Source
gf	85.68	kJ/mol	Joback Method
hf	-1196.29	kJ/mol	Joback Method
hfus	112.50	kJ/mol	Joback Method
hvap	122.69	kJ/mol	Joback Method
log10ws	-17.10		Crippen Method
logp	16.173		Crippen Method
mcvol	638.260	ml/mol	McGowan Method
pc	343.44	kPa	Joback Method
rinpol	4547.32		NIST Webbook
rinpol	4547.32		NIST Webbook
tb	1282.41	K	Joback Method
tc	1897.39	K	Joback Method
tf	657.80	K	Joback Method
vc	2.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	2506.20	J/mol×K	1282.41	Joback Method
cpg	2558.71	J/mol×K	1384.91	Joback Method
cpg	2603.30	J/mol×K	1487.40	Joback Method
cpg	2642.88	J/mol×K	1589.90	Joback Method
cpg	2680.35	J/mol×K	1692.40	Joback Method
cpg	2718.60	J/mol×K	1794.89	Joback Method
cpg	2760.54	J/mol×K	1897.39	Joback Method
dvisc	0.0000595	Pa×s	657.80	Joback Method
dvisc	0.0000219	Pa×s	761.90	Joback Method
dvisc	0.0000102	Pa×s	866.00	Joback Method
dvisc	0.0000056	Pa×s	970.11	Joback Method
dvisc	0.0000035	Pa×s	1074.21	Joback Method
dvisc	0.0000023	Pa×s	1178.31	Joback Method
dvisc	0.0000017	Pa×s	1282.41	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=C17671271&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