Di-n-octadecyl sebacate

Inchi: InChI=1S/C46H90O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-31-35-39-43-49-45(47)41-
InchiKey: NTUPDNAURMTJID-UHFFFAOYSA-N
Formula: C46H90O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 707.20
CAS: 3072-03-5

Physical Properties

Property code	Value	Unit	Source
gf	-131.40	kJ/mol	Joback Method
hf	-1482.37	kJ/mol	Joback Method
hfus	120.47	kJ/mol	Joback Method
hvap	197.70 ± 6.90	kJ/mol	NIST Webbook
log10ws	-16.80		Crippen Method
logp	15.717		Crippen Method
mcvol	673.880	ml/mol	McGowan Method
pc	325.59	kPa	Joback Method
tb	1404.46	K	Joback Method
tc	2283.25	K	Joback Method
tf	752.50	K	Joback Method
vc	2.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2667.84	J/mol×K	1404.46	Joback Method
cpg	2713.41	J/mol×K	1550.92	Joback Method
cpg	2745.32	J/mol×K	1697.39	Joback Method
cpg	2771.27	J/mol×K	1843.85	Joback Method
cpg	2798.95	J/mol×K	1990.32	Joback Method
cpg	2836.08	J/mol×K	2136.78	Joback Method
cpg	2890.35	J/mol×K	2283.25	Joback Method
cpl	1481.00	J/mol×K	353.00	NIST Webbook
dvisc	0.0000212	Pa×s	752.50	Joback Method

dvisc	0.0000086	Pa×s	861.16	Joback Method
dvisc	0.0000043	Pa×s	969.82	Joback Method
dvisc	0.0000024	Pa×s	1078.48	Joback Method
dvisc	0.0000015	Pa×s	1187.14	Joback Method
dvisc	0.0000011	Pa×s	1295.80	Joback Method
dvisc	0.0000008	Pa×s	1404.46	Joback Method
hvapt	157.50	kJ/mol	480.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3072035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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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