

Di-n-hexadecyl sebacate

Inchi:	InChI=1S/C42H82O4/c1-3-5-7-9-11-13-15-17-19-21-23-27-31-35-39-45-41(43)37-33-29-
InchiKey:	QTDJUGJAGNDLKQ-UHFFFAOYSA-N
Formula:	C42H82O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	651.10
CAS:	26719-48-2

Physical Properties

Property code	Value	Unit	Source
gf	-165.08	kJ/mol	Joback Method
hf	-1399.81	kJ/mol	Joback Method
hfus	110.11	kJ/mol	Joback Method
hvap	183.80 ± 6.40	kJ/mol	NIST Webbook
log10ws	-15.13		Crippen Method
logp	14.156		Crippen Method
mcvol	617.520	ml/mol	McGowan Method
pc	375.87	kPa	Joback Method
tb	1312.94	K	Joback Method
tc	1938.48	K	Joback Method
tf	707.42	K	Joback Method
vc	2.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2401.10	J/molxK	1312.94	Joback Method
cpg	2439.19	J/molxK	1417.20	Joback Method
cpg	2467.13	J/molxK	1521.45	Joback Method
cpg	2487.37	J/molxK	1625.71	Joback Method
cpg	2502.37	J/molxK	1729.97	Joback Method
cpg	2514.57	J/molxK	1834.22	Joback Method
cpg	2526.43	J/molxK	1938.48	Joback Method
cpl	1460.00	J/molxK	353.00	NIST Webbook
dvisc	0.0000401	Paxs	707.42	Joback Method

dvisc	0.0000166	Paxs	808.34	Joback Method
dvisc	0.0000083	Paxs	909.26	Joback Method
dvisc	0.0000048	Paxs	1010.18	Joback Method
dvisc	0.0000031	Paxs	1111.10	Joback Method
dvisc	0.0000021	Paxs	1212.02	Joback Method
dvisc	0.0000015	Paxs	1312.94	Joback Method
hvapt	149.80	kJ/mol	460.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C26719482&Units=SI

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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