Sebacic acid, heptyl hexadecyl ester

Inchi: InChI=1S/C33H64O4/c1-3-5-7-9-10-11-12-13-14-15-16-19-23-27-31-37-33(35)29-25-21-
InchiKey: XCODJHVTLOJEIE-UHFFFAOYSA-N
Formula: C33H64O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 524.86

Physical Properties

Property code	Value	Unit	Source
gf	-240.86	kJ/mol	Joback Method
hf	-1214.05	kJ/mol	Joback Method
hfus	86.80	kJ/mol	Joback Method
hvap	107.36	kJ/mol	Joback Method
log10ws	-11.36		Crippen Method
logp	10.645		Crippen Method
mcvol	490.710	ml/mol	McGowan Method
pc	542.35	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		NIST Webbook
tb	1107.02	K	Joback Method
tc	1427.61	K	Joback Method
tf	605.99	K	Joback Method
vc	1.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.85	J/mol×K	1107.02	Joback Method
cpg	1829.93	J/mol×K	1160.45	Joback Method
cpg	1853.43	J/mol×K	1213.88	Joback Method
cpg	1873.58	J/mol×K	1267.32	Joback Method
cpg	1890.60	J/mol×K	1320.75	Joback Method
cpg	1904.73	J/mol×K	1374.18	Joback Method
cpg	1916.20	J/mol×K	1427.61	Joback Method
dvisc	0.0001562	Pa×s	605.99	Joback Method

dvisc	0.0000681	Pa×s	689.50	Joback Method
dvisc	0.0000355	Pa×s	773.00	Joback Method
dvisc	0.0000210	Pa×s	856.50	Joback Method
dvisc	0.0000137	Pa×s	940.01	Joback Method
dvisc	0.0000095	Pa×s	1023.51	Joback Method
dvisc	0.0000070	Pa×s	1107.02	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=U354313&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