Decyl octyl adipate

Other names:	Hexanedioic acid, decyl octyl ester
	Adipic acid, decyl octyl ester
	Octyl decyl adipate
Inchi:	InChI=1S/C24H46O4/c1-3-5-7-9-11-12-14-18-22-28-24(26)20-16-15-19-23(25)27-21-17-
InchiKey:	NWSGBTCJMJADLE-UHFFFAOYSA-N
Formula:	C24H46O4
SMILES:	CCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	398.62
CAS:	110-29-2

Physical Properties

Property code	Value	Unit	Source
gf	-316.64	kJ/mol	Joback Method
hf	-1028.29	kJ/mol	Joback Method
hfus	63.49	kJ/mol	Joback Method
hvap	87.33	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	7.134		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	849.99	kPa	Joback Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook
tb	901.10	K	Joback Method
tc	1104.70	K	Joback Method
tf	504.56	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1217.58	J/mol×K	901.10	Joback Method
cpg	1304.84	J/mol×K	1070.77	Joback Method
cpg	1290.07	J/mol×K	1036.83	Joback Method

cpg	1273.99	J/mol×K	1002.90	Joback Method
cpg	1256.57	J/mol×K	968.97	Joback Method
cpg	1237.78	J/mol×K	935.03	Joback Method
cpg	1318.35	J/mol×K	1104.70	Joback Method
dvisc	0.0000294	Pa×s	901.10	Joback Method
dvisc	0.0000393	Pa×s	835.01	Joback Method
dvisc	0.0000553	Pa×s	768.92	Joback Method
dvisc	0.0000828	Pa×s	702.83	Joback Method
dvisc	0.0001350	Pa×s	636.74	Joback Method
dvisc	0.0002463	Pa×s	570.65	Joback Method
dvisc	0.0005261	Pa×s	504.56	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C110292&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
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