Diisooctyl adipate

Other names:	Hexanedioic acid, diisooctyl ester
	Monoplex DIOA
	Plasthall DIOA
Inchi:	InChI=1S/C22H42O4/c1-19(2)13-7-5-11-17-25-21(23)15-9-10-16-22(24)26-18-12-6-8-14
InchiKey:	CJFLBOQMPJCWLR-UHFFFAOYSA-N
Formula:	C22H42O4
SMILES:	CC(C)CCCCCOC(=O)CCCCC(=O)OCCCCCC(C)C
Mol. weight [g/mol]:	370.57
CAS:	1330-86-5

Physical Properties

Property code	Value	Unit	Source
gf	-338.36	kJ/mol	Joback Method
hf	-997.57	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	6.066		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	963.27	kPa	Joback Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1980.00		NIST Webbook
tb	854.46	K	Joback Method
tc	1046.57	K	Joback Method
tf	452.02	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1092.98	J/mol×K	854.46	Joback Method
cpg	1176.86	J/mol×K	1014.55	Joback Method
cpg	1162.43	J/mol×K	982.53	Joback Method
cpg	1146.85	J/mol×K	950.51	Joback Method
cpg	1130.10	J/mol×K	918.50	Joback Method
cpg	1112.15	J/mol×K	886.48	Joback Method
cpg	1190.16	J/mol×K	1046.57	Joback Method
dvisc	0.0000333	Pa×s	854.46	Joback Method
dvisc	0.0000458	Pa×s	787.39	Joback Method
dvisc	0.0000669	Pa×s	720.31	Joback Method
dvisc	0.0001055	Pa×s	653.24	Joback Method
dvisc	0.0001845	Pa×s	586.17	Joback Method
dvisc	0.0003731	Pa×s	519.09	Joback Method
dvisc	0.0009298	Pa×s	452.02	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1330865&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume