DIISODECYL ADIPATE

Other names: Hexanedioic acid, diisodecyl ester
Kodaflex DIDA
Monoplex DDA
Plasthall DIDA
Inchi: InChI=1S/C26H50O4/c1-23(2)17-11-7-5-9-15-21-29-25(27)19-13-14-20-26(28)30-22-16-
InchiKey: YKGYQYOQRGPFTO-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CC(C)CCCCCCCOC(=O)CCCCC(=O)OCCCCCCCC(C)C
Mol. weight [g/mol]: 426.68

Physical Properties

Property code	Value	Unit	Source
af	1.1998		Cheméo Relay (1.0)
hf	-1221.29	kJ/mol	Cheméo Relay (1.0)
hfus	61.62	kJ/mol	Joback Method
hvap	116.03	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.98		Cheméo Relay (1.0)
logp	7.626		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	769.04	kPa	Joback Method
rinpol	2745.00		NIST Webbook
rinpol	2782.00		NIST Webbook
rinpol	2745.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	652.74	K	Cheméo Relay (1.0)
tc	820.51	K	Cheméo Relay (1.0)
tf	294.96	K	Cheméo Relay (1.0)
vc	1.506	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.96	J/mol×K	945.98	Joback Method
cpg	1448.19	J/mol×K	1162.69	Joback Method

cpg	1435.00	J/mol×K	1126.57	Joback Method
cpg	1420.33	J/mol×K	1090.45	Joback Method
cpg	1404.14	J/mol×K	1054.33	Joback Method
cpg	1386.38	J/mol×K	1018.22	Joback Method
cpg	1367.00	J/mol×K	982.10	Joback Method
dvisc	0.0000581	Pa×s	721.54	Joback Method
dvisc	0.0000180	Pa×s	945.98	Joback Method
dvisc	0.0000248	Pa×s	871.17	Joback Method
dvisc	0.0000365	Pa×s	796.35	Joback Method
dvisc	0.0005428	Pa×s	497.10	Joback Method
dvisc	0.0001030	Pa×s	646.73	Joback Method
dvisc	0.0002121	Pa×s	571.91	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27178161&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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