Hexanedioic acid, diheptyl ester

Other names: diheptyl adipate
adipic acid, diheptyl ester
Inchi: InChI=1S/C20H38O4/c1-3-5-7-9-13-17-23-19(21)15-11-12-16-20(22)24-18-14-10-8-6-4-2
InchiKey: SITULKFUBJXOJH-UHFFFAOYSA-N
Formula: C20H38O4
SMILES: CCCCCCCOC(=O)CCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 342.51
CAS: 14697-48-4

Physical Properties

Property code	Value	Unit	Source
gf	-350.32	kJ/mol	Joback Method
hf	-945.73	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.574		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1077.81	kPa	Joback Method
rinpol	2331.00		NIST Webbook
tb	809.58	K	Joback Method
tc	993.33	K	Joback Method
tf	459.48	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.18	J/mol×K	809.58	Joback Method
cpg	987.44	J/mol×K	840.20	Joback Method
cpg	1004.65	J/mol×K	870.83	Joback Method
cpg	1020.84	J/mol×K	901.45	Joback Method
cpg	1036.02	J/mol×K	932.08	Joback Method
cpg	1050.21	J/mol×K	962.70	Joback Method

cpg	1063.43	J/mol×K	993.33	Joback Method
dvisc	0.0008397	Pa×s	459.48	Joback Method
dvisc	0.0004093	Pa×s	517.83	Joback Method
dvisc	0.0002308	Pa×s	576.18	Joback Method
dvisc	0.0001446	Pa×s	634.53	Joback Method
dvisc	0.0000980	Pa×s	692.88	Joback Method
dvisc	0.0000706	Pa×s	751.23	Joback Method
dvisc	0.0000533	Pa×s	809.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14697484&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

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