Adipic acid, di(3-heptyl) ester

Other names: di-(1-Ethylpentyl)adipate
Inchi: InChI=1S/C20H38O4/c1-5-9-13-17(7-3)23-19(21)15-11-12-16-20(22)24-18(8-4)14-10-6-2
InchiKey: HBNOQOBSGMHAMR-UHFFFAOYSA-N
Formula: C20H38O4
SMILES: CCCCC(CC)OC(=O)CCCCC(=O)OC(CC)CCCC
Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-355.20	kJ/mol	Joback Method
hf	-956.29	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	77.65	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.571		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
rinpol	2113.00		NIST Webbook
rinpol	2131.00		NIST Webbook
tb	808.70	K	Joback Method
tc	994.02	K	Joback Method
tf	429.48	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.14	J/mol×K	808.70	Joback Method
cpg	1051.61	J/mol×K	963.13	Joback Method
cpg	1037.40	J/mol×K	932.24	Joback Method
cpg	1022.17	J/mol×K	901.36	Joback Method
cpg	1005.89	J/mol×K	870.47	Joback Method
cpg	988.55	J/mol×K	839.59	Joback Method
cpg	1064.82	J/mol×K	994.02	Joback Method

dvisc	0.0000449	Pa×s	808.70	Joback Method
dvisc	0.0000615	Pa×s	745.50	Joback Method
dvisc	0.0000894	Pa×s	682.29	Joback Method
dvisc	0.0001402	Pa×s	619.09	Joback Method
dvisc	0.0002435	Pa×s	555.89	Joback Method
dvisc	0.0004873	Pa×s	492.68	Joback Method
dvisc	0.0011959	Pa×s	429.48	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=U353664&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume