

Adipic acid, 3-heptyl isoheptyl ester

Inchi:	InChI=1S/C19H36O4/c1-5-7-12-17(6-2)23-19(21)14-9-8-13-18(20)22-15-10-11-16(3)4/h1
InchiKey:	LYLBCTVAZAUWTQ-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCCCC(CC)OC(=O)CCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	328.49

Physical Properties

Property code	Value	Unit	Source
gf	-363.62	kJ/mol	Joback Method
hf	-935.65	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.038		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	785.82	K	Joback Method
tc	968.88	K	Joback Method
tf	418.21	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.87	J/mol×K	785.82	Joback Method
cpg	990.13	J/mol×K	938.37	Joback Method
cpg	976.05	J/mol×K	907.86	Joback Method
cpg	961.00	J/mol×K	877.35	Joback Method
cpg	944.96	J/mol×K	846.84	Joback Method
cpg	927.92	J/mol×K	816.33	Joback Method
cpg	1003.26	J/mol×K	968.88	Joback Method
dvisc	0.0000520	Paxs	785.82	Joback Method

dvisc	0.0000711	Paxs	724.55	Joback Method
dvisc	0.0001030	Paxs	663.28	Joback Method
dvisc	0.0001610	Paxs	602.01	Joback Method
dvisc	0.0002785	Paxs	540.75	Joback Method
dvisc	0.0005543	Paxs	479.48	Joback Method
dvisc	0.0013492	Paxs	418.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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