

Adipic acid, butyl 10-chlorodecyl ester

Inchi:	InChI=1S/C20H37ClO4/c1-2-3-17-24-19(22)14-10-11-15-20(23)25-18-13-9-7-5-4-6-8-12
InchiKey:	ZHDPBMMHKUYQOC-UHFFFAOYSA-N
Formula:	C20H37ClO4
SMILES:	CCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCI
Mol. weight [g/mol]:	376.96

Physical Properties

Property code	Value	Unit	Source
gf	-362.25	kJ/mol	Joback Method
hf	-961.47	kJ/mol	Joback Method
hfus	57.33	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.793		Crippen Method
mcvol	319.780	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2654.00		NIST Webbook
tb	847.01	K	Joback Method
tc	1037.90	K	Joback Method
tf	489.40	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.82	J/mol×K	847.01	Joback Method
cpg	1018.18	J/mol×K	878.83	Joback Method
cpg	1034.44	J/mol×K	910.64	Joback Method
cpg	1049.64	J/mol×K	942.46	Joback Method
cpg	1063.78	J/mol×K	974.27	Joback Method
cpg	1076.89	J/mol×K	1006.09	Joback Method
cpg	1088.99	J/mol×K	1037.90	Joback Method
dvisc	0.0006619	Pa×s	489.40	Joback Method
dvisc	0.0003326	Pa×s	549.00	Joback Method

dvisc	0.0001913	Pa×s	608.60	Joback Method
dvisc	0.0001214	Pa×s	668.20	Joback Method
dvisc	0.0000830	Pa×s	727.81	Joback Method
dvisc	0.0000601	Pa×s	787.41	Joback Method
dvisc	0.0000456	Pa×s	847.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353487&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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