

butyl (Z,Z)-9,12-octadecadienoate

Inchi:	InChI=1S/C22H40O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22(23)24-21-6-4-2
InchiKey:	SVGGKWILBMPIJV-UTJQPWESSA-N
Formula:	C22H40O2
SMILES:	CCCCC=CCC=CCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	336.55

Physical Properties

Property code	Value	Unit	Source
gf	60.88	kJ/mol	Joback Method
hf	-507.77	kJ/mol	Joback Method
hfus	55.93	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	7.143		Crippen Method
mvol	319.680	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
ripol	2631.00		NIST Webbook
ripol	2631.00		NIST Webbook
tb	787.37	K	Joback Method
tc	968.88	K	Joback Method
tf	399.70	K	Joback Method
vc	1.252	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.44	J/molxK	787.37	Joback Method
cpg	1001.90	J/molxK	817.62	Joback Method
cpg	1020.40	J/molxK	847.87	Joback Method
cpg	1038.00	J/molxK	878.13	Joback Method
cpg	1054.74	J/molxK	908.38	Joback Method
cpg	1070.67	J/molxK	938.63	Joback Method
cpg	1085.84	J/molxK	968.88	Joback Method
dvisc	0.0011728	Paxs	399.70	Joback Method

dvisc	0.0004577	Paxs	464.31	Joback Method
dvisc	0.0002248	Paxs	528.92	Joback Method
dvisc	0.0001289	Paxs	593.53	Joback Method
dvisc	0.0000824	Paxs	658.15	Joback Method
dvisc	0.0000571	Paxs	722.76	Joback Method
dvisc	0.0000420	Paxs	787.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301601&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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