

butyl nonacosanoate

Inchi: InChI=1S/C33H66O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey: JXXYQWVJJWZEJD-UHFFFAOYSA-N
Formula: C33H66O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]: 494.88

Physical Properties

Property code	Value	Unit	Source
gf	-6.94	kJ/mol	Joback Method
hf	-969.25	kJ/mol	Joback Method
hfus	84.01	kJ/mol	Joback Method
hvap	98.21	kJ/mol	Joback Method
log10ws	-12.50		Crippen Method
logp	11.882		Crippen Method
mvol	483.270	ml/mol	McGowan Method
pc	530.91	kPa	Joback Method
rinpol	3475.19		NIST Webbook
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tb	1030.73	K	Joback Method
tc	1306.79	K	Joback Method
tf	533.83	K	Joback Method
vc	1.907	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1750.75	J/molxK	1030.73	Joback Method
cpg	1780.48	J/molxK	1076.74	Joback Method
cpg	1807.60	J/molxK	1122.75	Joback Method
cpg	1832.30	J/molxK	1168.76	Joback Method
cpg	1854.77	J/molxK	1214.77	Joback Method
cpg	1875.18	J/molxK	1260.78	Joback Method
cpg	1893.74	J/molxK	1306.79	Joback Method
dvisc	0.0003193	Paxs	533.83	Joback Method

dvisc	0.0001232	Paxs	616.65	Joback Method
dvisc	0.0000595	Paxs	699.46	Joback Method
dvisc	0.0000336	Paxs	782.28	Joback Method
dvisc	0.0000211	Paxs	865.10	Joback Method
dvisc	0.0000144	Paxs	947.91	Joback Method
dvisc	0.0000105	Paxs	1030.73	Joback Method

Sources

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=R437433&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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