

Heneicosanoic acid, butyl ester

Other names:	Butyl heneicosanoate
Inchi:	InChI=1S/C25H50O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25(26)2
InchiKey:	XZWLWKJMSBKVEW-UHFFFAOYSA-N
Formula:	C25H50O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	382.66

Physical Properties

Property code	Value	Unit	Source
gf	-74.30	kJ/mol	Joback Method
hf	-804.13	kJ/mol	Joback Method
hfus	63.29	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	8.762		Crippen Method
mcvol	370.550	ml/mol	McGowan Method
pc	783.75	kPa	Joback Method
rinpol	2676.00		NIST Webbook
tb	847.69	K	Joback Method
tc	1038.15	K	Joback Method
tf	443.67	K	Joback Method
vc	1.460	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.77	J/molxK	847.69	Joback Method
cpg	1243.05	J/molxK	879.43	Joback Method
cpg	1264.07	J/molxK	911.18	Joback Method
cpg	1283.89	J/molxK	942.92	Joback Method
cpg	1302.54	J/molxK	974.66	Joback Method
cpg	1320.07	J/molxK	1006.41	Joback Method
cpg	1336.53	J/molxK	1038.15	Joback Method
dvisc	0.0009384	Paxs	443.67	Joback Method

dvisc	0.0003813	Paxs	511.01	Joback Method
dvisc	0.0001910	Paxs	578.34	Joback Method
dvisc	0.0001106	Paxs	645.68	Joback Method
dvisc	0.0000710	Paxs	713.02	Joback Method
dvisc	0.0000492	Paxs	780.35	Joback Method
dvisc	0.0000361	Paxs	847.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405180&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

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