

Eicosanoic acid, isobutyl ester

Other names:	Isobutyl arachidate
Inchi:	InChI=1S/C24H48O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24(25)26-22
InchiKey:	WKVHKJPNBFWXHD-UHFFFAOYSA-N
Formula:	C24H48O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	368.64

Physical Properties

Property code	Value	Unit	Source
gf	-85.16	kJ/mol	Joback Method
hf	-788.77	kJ/mol	Joback Method
hfus	57.18	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	8.227		Crippen Method
mvol	356.460	ml/mol	McGowan Method
pc	831.46	kPa	Joback Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook
tb	824.37	K	Joback Method
tc	1009.38	K	Joback Method
tf	417.40	K	Joback Method
vc	1.397	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.23	J/mol×K	824.37	Joback Method
cpg	1178.90	J/mol×K	855.21	Joback Method
cpg	1199.39	J/mol×K	886.04	Joback Method
cpg	1218.75	J/mol×K	916.88	Joback Method
cpg	1237.01	J/mol×K	947.71	Joback Method
cpg	1254.21	J/mol×K	978.55	Joback Method
cpg	1270.38	J/mol×K	1009.38	Joback Method

dvisc	0.0012961	Paxs	417.40	Joback Method
dvisc	0.0004783	Paxs	485.23	Joback Method
dvisc	0.0002254	Paxs	553.06	Joback Method
dvisc	0.0001252	Paxs	620.88	Joback Method
dvisc	0.0000781	Paxs	688.71	Joback Method
dvisc	0.0000530	Paxs	756.54	Joback Method
dvisc	0.0000384	Paxs	824.37	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=U405169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	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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