

Fumaric acid, 2-butyl undecyl ester

Inchi:	InChI=1S/C19H34O4/c1-4-6-7-8-9-10-11-12-13-16-22-18(20)14-15-19(21)23-17(3)5-2/h
InchiKey:	BHJPESYXXLVCMH-CCEZHUSRSA-N
Formula:	C19H34O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CC
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-280.96	kJ/mol	Joback Method
hf	-813.15	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.958		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	790.42	K	Joback Method
tc	975.43	K	Joback Method
tf	428.13	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.58	J/molxK	790.42	Joback Method
cpg	901.98	J/molxK	821.26	Joback Method
cpg	918.41	J/molxK	852.09	Joback Method
cpg	933.89	J/molxK	882.93	Joback Method
cpg	948.47	J/molxK	913.76	Joback Method
cpg	962.14	J/molxK	944.60	Joback Method
cpg	974.95	J/molxK	975.43	Joback Method
dvisc	0.0010369	Paxs	428.13	Joback Method

dvisc	0.0004554	Paxs	488.51	Joback Method
dvisc	0.0002397	Paxs	548.89	Joback Method
dvisc	0.0001433	Paxs	609.27	Joback Method
dvisc	0.0000940	Paxs	669.66	Joback Method
dvisc	0.0000661	Paxs	730.04	Joback Method
dvisc	0.0000490	Paxs	790.42	Joback Method

Sources

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=U348648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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