

Fumaric acid, butyl tridecyl ester

Inchi:	InChI=1S/C21H38O4/c1-3-5-7-8-9-10-11-12-13-14-15-19-25-21(23)17-16-20(22)24-18-6
InchiKey:	QSXWKTIUGHXXMP-WUKNDPDISA-N
Formula:	C21H38O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OCCCC
Mol. weight [g/mol]:	354.52

Physical Properties

Property code	Value	Unit	Source
gf	-261.68	kJ/mol	Joback Method
hf	-849.15	kJ/mol	Joback Method
hfus	55.92	kJ/mol	Joback Method
hvap	80.61	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.740		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1047.33	kPa	Joback Method
rinqol	2485.00		NIST Webbook
tb	836.62	K	Joback Method
tc	1025.83	K	Joback Method
tf	465.67	K	Joback Method
vc	1.240	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.47	J/molxK	836.62	Joback Method
cpg	1084.75	J/molxK	994.30	Joback Method
cpg	1070.69	J/molxK	962.76	Joback Method
cpg	1055.65	J/molxK	931.23	Joback Method
cpg	1039.63	J/molxK	899.69	Joback Method
cpg	1022.57	J/molxK	868.16	Joback Method
cpg	1097.88	J/molxK	1025.83	Joback Method
dvisc	0.0000401	Paxs	836.62	Joback Method
dvisc	0.0000534	Paxs	774.80	Joback Method

dvisc	0.0000747	Paxs	712.97	Joback Method
dvisc	0.0001114	Paxs	651.14	Joback Method
dvisc	0.0001807	Paxs	589.32	Joback Method
dvisc	0.0003282	Paxs	527.50	Joback Method
dvisc	0.0006985	Paxs	465.67	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=U348804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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