Fumaric acid, 2-butyl eicosyl ester

Inchi: InChI=1S/C28H52O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-31-27(2
InchiKey: KROOSDKWDJWJIS-WCWDXBQESA-N
Formula: C28H52O4
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CC
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-205.18	kJ/mol	Joback Method
hf	-998.91	kJ/mol	Joback Method
hfus	70.53	kJ/mol	Joback Method
hvap	95.80	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	8.469		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	709.60	kPa	Joback Method
rinpol	3122.00		NIST Webbook
rinpol	3122.00		NIST Webbook
tb	996.34	K	Joback Method
tc	1231.91	K	Joback Method
tf	529.56	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.75	J/mol×K	996.34	Joback Method
cpg	1468.66	J/mol×K	1035.60	Joback Method
cpg	1488.79	J/mol×K	1074.86	Joback Method
cpg	1507.22	J/mol×K	1114.12	Joback Method
cpg	1524.05	J/mol×K	1153.39	Joback Method
cpg	1539.36	J/mol×K	1192.65	Joback Method
cpg	1553.25	J/mol×K	1231.91	Joback Method
dvisc	0.0003320	Pa×s	529.56	Joback Method

dvisc	0.0001357	Pa×s	607.36	Joback Method
dvisc	0.0000680	Pa×s	685.15	Joback Method
dvisc	0.0000392	Pa×s	762.95	Joback Method
dvisc	0.0000250	Pa×s	840.75	Joback Method
dvisc	0.0000173	Pa×s	918.54	Joback Method
dvisc	0.0000126	Pa×s	996.34	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=U348656&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