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: CCCCCCCCCCCCCOC(=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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000747	Pa×s	712.97	Joback Method
dvisc	0.0001114	Pa×s	651.14	Joback Method
dvisc	0.0001807	Pa×s	589.32	Joback Method
dvisc	0.0003282	Pa×s	527.50	Joback Method
dvisc	0.0006985	Pa×s	465.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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