Fumaric acid, 2-methylpent-3-yl octadecyl ester

Inchi: InChI=1S/C28H52O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-31-27(29)22-
InchiKey: NPLHVCCTMWOIOI-GHVJWSGMSA-N
Formula: C28H52O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-207.62	kJ/mol	Joback Method
hf	-1004.19	kJ/mol	Joback Method
hfus	67.01	kJ/mol	Joback Method
hvap	95.42	kJ/mol	Joback Method
log10ws	-8.99		Crippen Method
logp	8.325		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	712.63	kPa	Joback Method
rinpol	3073.00		NIST Webbook
rinpol	3073.00		NIST Webbook
tb	995.90	K	Joback Method
tc	1229.46	K	Joback Method
tf	514.56	K	Joback Method
vc	1.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1447.04	J/mol×K	995.90	Joback Method
cpg	1468.71	J/mol×K	1034.83	Joback Method
cpg	1488.61	J/mol×K	1073.75	Joback Method
cpg	1506.83	J/mol×K	1112.68	Joback Method
cpg	1523.45	J/mol×K	1151.60	Joback Method
cpg	1538.56	J/mol×K	1190.53	Joback Method
cpg	1552.25	J/mol×K	1229.46	Joback Method
dvisc	0.0003830	Pa×s	514.56	Joback Method

dvisc	0.0001439	Pa×s	594.78	Joback Method
dvisc	0.0000682	Pa×s	675.01	Joback Method
dvisc	0.0000379	Pa×s	755.23	Joback Method
dvisc	0.0000236	Pa×s	835.45	Joback Method
dvisc	0.0000159	Pa×s	915.68	Joback Method
dvisc	0.0000115	Pa×s	995.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348774&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

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