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

Inchi: InChI=1S/C28H52O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-31-26(29)22-
InchiKey: JQOWQHQKOMWCID-GHVJWSGMSA-N
Formula: C28H52O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-202.34	kJ/mol	Joback Method
hf	-1007.66	kJ/mol	Joback Method
hfus	63.12	kJ/mol	Joback Method
hvap	94.51	kJ/mol	Joback Method
log10ws	-8.99		Crippen Method
logp	8.325		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	716.83	kPa	Joback Method
rinpol	3044.00		NIST Webbook
rinpol	3044.00		NIST Webbook
tb	993.11	K	Joback Method
tc	1222.73	K	Joback Method
tf	531.98	K	Joback Method
vc	1.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.35	J/mol×K	993.11	Joback Method
cpg	1539.32	J/mol×K	1184.46	Joback Method
cpg	1523.41	J/mol×K	1146.19	Joback Method
cpg	1506.26	J/mol×K	1107.92	Joback Method
cpg	1487.77	J/mol×K	1069.65	Joback Method
cpg	1467.84	J/mol×K	1031.38	Joback Method
cpg	1554.10	J/mol×K	1222.73	Joback Method
dvisc	0.0000095	Pa×s	993.11	Joback Method

dvisc	0.0000133	Pa×s	916.26	Joback Method
dvisc	0.0000197	Pa×s	839.40	Joback Method
dvisc	0.0000316	Pa×s	762.55	Joback Method
dvisc	0.0000564	Pa×s	685.69	Joback Method
dvisc	0.0001164	Pa×s	608.84	Joback Method
dvisc	0.0002963	Pa×s	531.98	Joback Method

Sources

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=U348717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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