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

Inchi: InChI=1S/C25H46O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-21-28-23(26)19-20-24(27)

InchiKey: ODIHJLXJDLHOBV-FMQUCBEESA-N

Formula: C25H46O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-227.60	kJ/mol	Joback Method
hf	-945.74	kJ/mol	Joback Method
hfus	55.34	kJ/mol	Joback Method
hvap	87.83	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	7.155		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	841.62	kPa	Joback Method
rinpol	2738.00		NIST Webbook
rinpol	2738.00		NIST Webbook
tb	924.47	K	Joback Method
tc	1131.98	K	Joback Method
tf	498.17	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1254.11	J/mol×K	924.47	Joback Method
cpg	1273.85	J/mol×K	959.06	Joback Method
cpg	1292.30	J/mol×K	993.64	Joback Method
cpg	1309.54	J/mol×K	1028.23	Joback Method
cpg	1325.63	J/mol×K	1062.81	Joback Method
cpg	1340.65	J/mol×K	1097.40	Joback Method
cpg	1354.65	J/mol×K	1131.98	Joback Method
dvisc	0.0004577	Pa×s	498.17	Joback Method

dvisc	0.0001832	Pa×s	569.22	Joback Method
dvisc	0.0000898	Pa×s	640.27	Joback Method
dvisc	0.0000508	Pa×s	711.32	Joback Method
dvisc	0.0000318	Pa×s	782.37	Joback Method
dvisc	0.0000216	Pa×s	853.42	Joback Method
dvisc	0.0000155	Pa×s	924.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348714&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