Fumaric acid, 2-decyl isobutyl ester

Inchi: InChI=1S/C18H32O4/c1-5-6-7-8-9-10-11-16(4)22-18(20)13-12-17(19)21-14-15(2)3/h12-1
InchiKey: IIUWHOOOIYSQHK-OUKQBFOZSA-N
Formula: C18H32O4
SMILES: CCCCCCCCC(C)OC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-291.82	kJ/mol	Joback Method
hf	-797.79	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	73.16	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.424		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	767.10	K	Joback Method
tc	952.42	K	Joback Method
tf	401.86	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.20	J/mol×K	767.10	Joback Method
cpg	902.91	J/mol×K	921.53	Joback Method
cpg	889.37	J/mol×K	890.65	Joback Method
cpg	874.95	J/mol×K	859.76	Joback Method
cpg	859.63	J/mol×K	828.87	Joback Method
cpg	843.39	J/mol×K	797.99	Joback Method
cpg	915.59	J/mol×K	952.42	Joback Method
dvisc	0.0000519	Pa×s	767.10	Joback Method

dvisc	0.0000711	Pa×s	706.23	Joback Method
dvisc	0.0001032	Pa×s	645.35	Joback Method
dvisc	0.0001620	Pa×s	584.48	Joback Method
dvisc	0.0002825	Pa×s	523.61	Joback Method
dvisc	0.0005699	Pa×s	462.73	Joback Method
dvisc	0.0014223	Pa×s	401.86	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=U348585&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