Fumaric acid, 4-heptyl octyl ester

Inchi: InChI=1S/C19H34O4/c1-4-7-8-9-10-11-16-22-18(20)14-15-19(21)23-17(12-5-2)13-6-3/h1
InchiKey: NSYLLJKCJKYHNX-CCEZHUSRSA-N
Formula: C19H34O4
SMILES: CCCCCCCCOC(=O)C=CC(=O)OC(CCC)CCC
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-280.96	kJ/mol	Joback Method
hf	-813.15	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.958		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	790.42	K	Joback Method
tc	975.43	K	Joback Method
tf	428.13	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.58	J/mol×K	790.42	Joback Method
cpg	901.98	J/mol×K	821.26	Joback Method
cpg	918.41	J/mol×K	852.09	Joback Method
cpg	933.89	J/mol×K	882.93	Joback Method
cpg	948.47	J/mol×K	913.76	Joback Method
cpg	962.14	J/mol×K	944.60	Joback Method
cpg	974.95	J/mol×K	975.43	Joback Method
dvisc	0.0010369	Pa×s	428.13	Joback Method

dvisc	0.0004554	Pa×s	488.51	Joback Method
dvisc	0.0002397	Pa×s	548.89	Joback Method
dvisc	0.0001433	Pa×s	609.27	Joback Method
dvisc	0.0000940	Pa×s	669.66	Joback Method
dvisc	0.0000661	Pa×s	730.04	Joback Method
dvisc	0.0000490	Pa×s	790.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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