Dihexyl fumarate

Other names:	di-n-Hexyl fumarate
	2-Butenedioic acid (E)-, dihexyl ester
	Fumaric acid, dihexyl ester
	Dihexyl trans-butenedioate
	Hexyl fumarate
Inchi:	InChI=1S/C16H28O4/c1-3-5-7-9-13-19-15(17)11-12-16(18)20-14-10-8-6-4-2/h11-12H,3-1
InchiKey:	QMCVOSQFZZCSLN-VAWYXSNFSA-N
Formula:	C16H28O4
SMILES:	CCCCCCOC(=O)C=CC(=O)OCCCCCC
Mol. weight [g/mol]:	284.39
CAS:	19139-31-2

Physical Properties

Property code	Value	Unit	Source
gf	-303.78	kJ/mol	Joback Method
hf	-745.95	kJ/mol	Joback Method
hfus	42.97	kJ/mol	Joback Method
hvap	69.48	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.790		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
tb	722.22	K	Joback Method
tc	902.85	K	Joback Method
tf	409.32	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.41	J/mol×K	722.22	Joback Method
cpg	782.74	J/mol×K	872.75	Joback Method
cpg	769.83	J/mol×K	842.64	Joback Method
cpg	756.16	J/mol×K	812.54	Joback Method

cpg	741.71	J/mol×K	782.43	Joback Method
cpg	726.47	J/mol×K	752.33	Joback Method
cpg	794.90	J/mol×K	902.85	Joback Method
dvisc	0.0000801	Pa×s	722.22	Joback Method
dvisc	0.0001051	Pa×s	670.07	Joback Method
dvisc	0.0001446	Pa×s	617.92	Joback Method
dvisc	0.0002109	Pa×s	565.77	Joback Method
dvisc	0.0003321	Pa×s	513.62	Joback Method
dvisc	0.0005794	Pa×s	461.47	Joback Method
dvisc	0.0011649	Pa×s	409.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.00 ± 1.00	K	0.80	NIST Webbook

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=C19139312&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume