Fumaric acid, heptyl trans-hex-3-enyl ester

Inchi: InChI=1S/C17H28O4/c1-3-5-7-9-11-15-21-17(19)13-12-16(18)20-14-10-8-6-4-2/h6,8,12-
InchiKey: BCEIUXPWGYTDGB-JQAHBYNNSA-N
Formula: C17H28O4
SMILES: CCC=CCCOC(=O)C=CC(=O)OCCCCCCC
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-215.14	kJ/mol	Joback Method
hf	-649.37	kJ/mol	Joback Method
hfus	45.76	kJ/mol	Joback Method
hvap	71.66	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.956		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		NIST Webbook
tb	749.26	K	Joback Method
tc	934.62	K	Joback Method
tf	415.51	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.30	J/mol×K	749.26	Joback Method
cpg	814.98	J/mol×K	903.72	Joback Method
cpg	802.20	J/mol×K	872.83	Joback Method
cpg	788.68	J/mol×K	841.94	Joback Method
cpg	774.37	J/mol×K	811.05	Joback Method
cpg	759.26	J/mol×K	780.15	Joback Method
cpg	827.02	J/mol×K	934.62	Joback Method
dvisc	0.0000607	Pa×s	749.26	Joback Method

dvisc	0.0000802	Pa×s	693.63	Joback Method
dvisc	0.0001112	Pa×s	638.01	Joback Method
dvisc	0.0001642	Pa×s	582.38	Joback Method
dvisc	0.0002631	Pa×s	526.76	Joback Method
dvisc	0.0004712	Pa×s	471.14	Joback Method
dvisc	0.0009864	Pa×s	415.51	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=U348888&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

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