

Fumaric acid, cis-hex-3-enyl heptyl 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-XXKCFVJZSA-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	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	749.26	K	Joback Method
tc	934.62	K	Joback Method
tf	415.51	K	Joback Method
vc	0.996	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000802	Paxs	693.63	Joback Method
dvisc	0.0001112	Paxs	638.01	Joback Method
dvisc	0.0001642	Paxs	582.38	Joback Method
dvisc	0.0002631	Paxs	526.76	Joback Method
dvisc	0.0004712	Paxs	471.14	Joback Method
dvisc	0.0009864	Paxs	415.51	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=U348863&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
mccvol:	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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