

Fumaric acid, heptyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C17H30O4/c1-5-6-7-8-9-12-20-16(18)10-11-17(19)21-15(4)13-14(2)3/h10-11,1
InchiKey: NFMFRPZBNLSLIH-ZHACJKMWSA-N
Formula: C17H30O4
SMILES: CCCCCCOC(=O)C=CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-300.24	kJ/mol	Joback Method
hf	-777.15	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	70.93	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.034		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	744.22	K	Joback Method
tc	929.08	K	Joback Method
tf	390.59	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.28	J/molxK	744.22	Joback Method
cpg	843.63	J/molxK	898.27	Joback Method
cpg	830.30	J/molxK	867.46	Joback Method
cpg	816.11	J/molxK	836.65	Joback Method
cpg	801.06	J/molxK	805.84	Joback Method
cpg	785.12	J/molxK	775.03	Joback Method
cpg	856.15	J/molxK	929.08	Joback Method
dvisc	0.0000596	Paxs	744.22	Joback Method

dvisc	0.0000815	Paxs	685.28	Joback Method
dvisc	0.0001181	Paxs	626.34	Joback Method
dvisc	0.0001847	Paxs	567.40	Joback Method
dvisc	0.0003206	Paxs	508.47	Joback Method
dvisc	0.0006432	Paxs	449.53	Joback Method
dvisc	0.0015918	Paxs	390.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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