

Fumaric acid, butyl 2-ethylphenyl ester

Inchi: InChI=1S/C16H20O4/c1-3-5-12-19-15(17)10-11-16(18)20-14-9-7-6-8-13(14)4-2/h6-11H,3
InchiKey: KSXSQWYDZYFTKX-ZHACJKMWSA-N
Formula: C16H20O4
SMILES: CCCOC(=O)C=CC(=O)Oc1ccccc1CC
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
gf	-201.00	kJ/mol	Joback Method
hf	-520.89	kJ/mol	Joback Method
hfus	36.62	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.054		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinqol	2020.00		NIST Webbook
tb	753.88	K	Joback Method
tc	961.93	K	Joback Method
tf	448.26	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.96	J/molxK	753.88	Joback Method
cpg	687.57	J/molxK	927.25	Joback Method
cpg	676.67	J/molxK	892.58	Joback Method
cpg	664.89	J/molxK	857.90	Joback Method
cpg	652.19	J/molxK	823.23	Joback Method
cpg	638.55	J/molxK	788.55	Joback Method
cpg	697.61	J/molxK	961.93	Joback Method
dvisc	0.0000809	Paxs	753.88	Joback Method
dvisc	0.0001030	Paxs	702.94	Joback Method

dvisc	0.0001362	Paxs	652.01	Joback Method
dvisc	0.0001887	Paxs	601.07	Joback Method
dvisc	0.0002779	Paxs	550.13	Joback Method
dvisc	0.0004428	Paxs	499.20	Joback Method
dvisc	0.0007844	Paxs	448.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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