

Fumaric acid, butyl 2,4-dimethylpent-3-yl ester

Inchi:	InChI=1S/C15H26O4/c1-6-7-10-18-13(16)8-9-14(17)19-15(11(2)3)12(4)5/h8-9,11-12,15H
InchiKey:	PWWSDFHFPYOXJO-CMDGGOBGSA-N
Formula:	C15H26O4
SMILES:	CCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-319.52	kJ/mol	Joback Method
hf	-741.15	kJ/mol	Joback Method
hfus	29.81	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.110		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpola	1726.00		NIST Webbook
tb	698.02	K	Joback Method
tc	886.19	K	Joback Method
tf	353.05	K	Joback Method
vc	0.885	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.12	J/molxK	698.02	Joback Method
cpg	672.46	J/molxK	729.38	Joback Method
cpg	687.94	J/molxK	760.74	Joback Method
cpg	702.57	J/molxK	792.10	Joback Method
cpg	716.37	J/molxK	823.46	Joback Method
cpg	729.35	J/molxK	854.82	Joback Method
cpg	741.53	J/molxK	886.19	Joback Method
dvisc	0.0025568	Paxs	353.05	Joback Method
dvisc	0.0009302	Paxs	410.55	Joback Method

dvisc	0.0004338	Paxs	468.04	Joback Method
dvisc	0.0002391	Paxs	525.53	Joback Method
dvisc	0.0001482	Paxs	583.03	Joback Method
dvisc	0.0001001	Paxs	640.52	Joback Method
dvisc	0.0000721	Paxs	698.02	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=U348544&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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