

Fumaric acid, 2-butyl heptyl ester

Inchi:	InChI=1S/C15H26O4/c1-4-6-7-8-9-12-18-14(16)10-11-15(17)19-13(3)5-2/h10-11,13H,4-9
InchiKey:	ZXLNOSGWPNTCY-ZHACJKMWSA-N
Formula:	C15H26O4
SMILES:	CCCCCCCOC(=O)C=CC(=O)OC(C)CC
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-314.64	kJ/mol	Joback Method
hf	-730.59	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.398		Crippen Method
mvol	232.790	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	698.90	K	Joback Method
tc	881.96	K	Joback Method
tf	383.05	K	Joback Method
vc	0.897	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.15	J/molxK	698.90	Joback Method
cpg	671.00	J/molxK	729.41	Joback Method
cpg	686.05	J/molxK	759.92	Joback Method
cpg	700.31	J/molxK	790.43	Joback Method
cpg	713.80	J/molxK	820.94	Joback Method
cpg	726.53	J/molxK	851.45	Joback Method
cpg	738.52	J/molxK	881.96	Joback Method
dvisc	0.0015587	Paxs	383.05	Joback Method

dvisc	0.0007144	Paxs	435.69	Joback Method
dvisc	0.0003874	Paxs	488.33	Joback Method
dvisc	0.0002366	Paxs	540.98	Joback Method
dvisc	0.0001578	Paxs	593.62	Joback Method
dvisc	0.0001124	Paxs	646.26	Joback Method
dvisc	0.0000842	Paxs	698.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348644&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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