Fumaric acid, butyl 4-heptyl ester

Inchi: InChI=1S/C15H26O4/c1-4-7-12-18-14(16)10-11-15(17)19-13(8-5-2)9-6-3/h10-11,13H,4-9
InchiKey: NNBUTFQSJGOBFJ-ZHACJKMWSA-N
Formula: C15H26O4
SMILES: CCCCOC(=O)C=CC(=O)OC(CCC)CCC
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
mcvol	232.790	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	1784.00		NIST Webbook
tb	698.90	K	Joback Method
tc	881.96	K	Joback Method
tf	383.05	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.15	J/mol×K	698.90	Joback Method
cpg	671.00	J/mol×K	729.41	Joback Method
cpg	686.05	J/mol×K	759.92	Joback Method
cpg	700.31	J/mol×K	790.43	Joback Method
cpg	713.80	J/mol×K	820.94	Joback Method
cpg	726.53	J/mol×K	851.45	Joback Method
cpg	738.52	J/mol×K	881.96	Joback Method
dvisc	0.0015587	Pa×s	383.05	Joback Method
dvisc	0.0007144	Pa×s	435.69	Joback Method

dvisc	0.0003874	Pa×s	488.33	Joback Method
dvisc	0.0002366	Pa×s	540.98	Joback Method
dvisc	0.0001578	Pa×s	593.62	Joback Method
dvisc	0.0001124	Pa×s	646.26	Joback Method
dvisc	0.0000842	Pa×s	698.90	Joback Method

Sources

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=U348513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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