

Fumaric acid, butyl 8-chlorooctyl ester

Inchi:	InChI=1S/C16H27ClO4/c1-2-3-13-20-15(18)10-11-16(19)21-14-9-7-5-4-6-8-12-17/h10-11
InchiKey:	PARYJXJJOSFHMQ-ZHACJKMWSA-N
Formula:	C16H27ClO4
SMILES:	CCCCOC(=O)C=CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]:	318.84

Physical Properties

Property code	Value	Unit	Source
gf	-315.71	kJ/mol	Joback Method
hf	-761.69	kJ/mol	Joback Method
hfus	47.17	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.008		Crippen Method
mvol	259.120	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	759.65	K	Joback Method
tc	945.22	K	Joback Method
tf	439.24	K	Joback Method
vc	1.008	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.46	J/molxK	759.65	Joback Method
cpg	755.65	J/molxK	790.58	Joback Method
cpg	770.00	J/molxK	821.51	Joback Method
cpg	783.54	J/molxK	852.44	Joback Method
cpg	796.28	J/molxK	883.37	Joback Method
cpg	808.24	J/molxK	914.29	Joback Method
cpg	819.45	J/molxK	945.22	Joback Method
dvisc	0.0009436	Paxs	439.24	Joback Method

dvisc	0.0004845	Paxs	492.64	Joback Method
dvisc	0.0002834	Paxs	546.04	Joback Method
dvisc	0.0001824	Paxs	599.44	Joback Method
dvisc	0.0001262	Paxs	652.85	Joback Method
dvisc	0.0000923	Paxs	706.25	Joback Method
dvisc	0.0000705	Paxs	759.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348530&Units=SI

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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