Fumaric acid, monoamide, N-(2-ethylphenyl)-, neopentyl ester

Inchi: InChI=1S/C17H23NO3/c1-5-13-8-6-7-9-14(13)18-15(19)10-11-16(20)21-12-17(2,3)4/h6-1

InchiKey: HVOIYMWCNJJVPM-ZHACJKMWSA-N

Formula: C17H23NO3

SMILES: CCc1ccccc1NC(=O)C=CC(=O)OCC(C)(C)C

Mol. weight [g/mol]: 289.37

Physical Properties

Property code	Value	Unit	Source
gf	4.65	kJ/mol	Joback Method
hf	-364.59	kJ/mol	Joback Method
hfus	35.71	kJ/mol	Joback Method
hvap	77.37	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.333		Crippen Method
mcvol	241.320	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	801.28	K	Joback Method
tc	1017.90	K	Joback Method
tf	492.38	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.23	J/mol×K	801.28	Joback Method
cpg	724.07	J/mol×K	837.38	Joback Method
cpg	737.88	J/mol×K	873.49	Joback Method
cpg	750.72	J/mol×K	909.59	Joback Method
cpg	762.67	J/mol×K	945.69	Joback Method
cpg	773.80	J/mol×K	981.80	Joback Method
cpg	784.18	J/mol×K	1017.90	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=U357514&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
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